

# Announcement Cover Page

**Federal Agency Name(s).**

U.S. Department of Energy  
Idaho Operations Office  
Procurement Services Division

**Funding Opportunity Title.**

Advanced Nuclear Research at Universities.

**Announcement Type.**

Initial Announcement

**Funding Opportunity Number.**

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**Catalog of Federal Domestic Assistance (CFDA) Number(s).**

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**CDFA Title(s).**

Nuclear Energy, Science and Technology, Department of Energy.

**Due Date(s).**

Letter of Intent: **N/A**

Pre-application: **N/A**

Application:

Due: Applications must have an IIPS transmission time stamp of not later than **5:00 p.m.**

**July 16, 2004.**

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# FULL ANNOUNCEMENT

## I. Funding Opportunity Description.

**BACKGROUND:** Since 1999, the Nuclear Energy Research Initiative (NERI) program has sponsored research to advance the state of nuclear science and technology in the United States by addressing the key technical issues impacting the expanded use of nuclear energy. The program has sponsored research and development on next-generation nuclear energy systems; proliferation resistant nuclear fuel cycle technologies; generation of hydrogen using nuclear power; improvements in light water reactor technology; and fundamental areas of nuclear science that directly impact the long-term success of nuclear energy. The advances in these areas are expected to be incorporated in potential future advanced reactor designs and nuclear fuel systems.

The NERI program has realized its goal of developing advanced nuclear energy systems and technology to help assure that the United States maintains a viable option to use nuclear energy to meet its energy and environmental needs. The research effort, conducted by the Nation's universities, laboratories, and industries, has helped maintain the nuclear research infrastructure in this country and has focused attention on the United States as a nuclear research and development leader. Research accomplishments include: reactor system and plant infrastructure concepts that utilize nuclear energy to produce hydrogen; new advanced controls, diagnostic techniques and information systems for potential use in automating future nuclear plants; advanced nuclear fuels that could allow higher burn-ups resulting in maximized energy production and improved plant economics; evaluation of direct energy conversion technologies for advanced nuclear power plants; and reactor physics data for advanced nuclear power systems. Through funding innovative nuclear research at the Nation's universities, the NERI program has also stimulated student enrollment in nuclear fields of study. Further highlights of the NERI program are contained in the *Nuclear Energy Research Initiative 2002 Annual Report* (see <http://neri.ne.doe.gov/>).

Beginning with this announcement, the NERI program is modified to focus on advanced nuclear research at the Nation's universities and integrated into the Department's mainline nuclear energy research and development (R&D) programs. The R&D conducted under this activity will directly support the Advanced Fuel Cycle Initiative (AFCI), the Generation IV Nuclear Energy Systems Initiative (Generation IV), and the Nuclear Hydrogen Initiative (NHI). A workshop was held March 4 and 5, 2004 in Gaithersburg Maryland to provide U.S. university researchers the opportunity to learn about these programs and how the new NERI program will operate. This announcement, which is open to all U.S. universities, provides an opportunity for universities to participate in these research initiatives. The NERI R&D projects will be selected using a competitive, peer-reviewed process. Funding for the NERI awards is provided by the AFCI, Generation IV, and NHI programs.

**OBJECTIVES:** The modified NERI program is intended to conduct R&D to meet the following objectives:

- Directly support the resolution of technical and scientific issues for the Advanced Fuel Cycle Initiative, the Generation IV Nuclear Energy Systems Initiative, and Nuclear Hydrogen Initiative programs;

- Integrate the Nation's universities into the Department's mainline nuclear R&D programs;
- Contribute to assuring a new generation of engineers and scientists for the nuclear future.

**SCOPE OF WORK:** The Department of Energy is seeking applications from universities for research and development (R&D) that will directly support its nuclear energy R&D in the Advanced Fuel Cycle Initiative (AFCI), Generation IV Nuclear Energy Systems Initiative (Generation IV), and Nuclear Hydrogen Initiative (NHI) programs. Information describing these programs, including detailed program and R&D plans and the proceedings of a recent workshop, may be found on the web at <http://neri.ne.doe.gov/publicinfo00.htm>, click on "Advanced Reactor, Fuel Cycle, and Energy Products Workshop for Universities, March 2004.", The program and program element schedules and milestones provided in these plans should be used as the basis of proposed project schedules, milestones, and deliverables. These three programs are organized into 17 program elements as follows:

- 1. Advanced Fuel Cycle Initiative**
  - 1.1 Spent Fuel Separations Technology
  - 1.2 Advanced Nuclear Fuel Development
  - 1.3 Transmutation Science and Engineering Technologies
  - 1.4 Advanced Fuel Cycle Systems Analysis
  - 1.5 Other AFCI Research
- 2. Generation IV Nuclear Energy Systems Initiative**
  - 2.1 Supercritical Water-Cooled Reactor
  - 2.2 Next Generation Nuclear Plant
  - 2.3 Lead Alloy Liquid-Metal-Cooled Fast Reactor
  - 2.4 Gas-Cooled Fast Reactor
  - 2.5 Design and Evaluation Methods Development
  - 2.6 Crosscutting Materials Development for Advanced Reactors
  - 2.7 Energy Conversion
  - 2.8 Other Generation IV Research
- 3. Nuclear Hydrogen Initiative**
  - 3.1 Thermochemical Cycles
  - 3.2 High Temperature Electrolysis
  - 3.3 Reactor-Hydrogen Production Process Interface
  - 3.4 Other Nuclear Hydrogen Production Research

A summary of the R&D needs in each of these program elements is discussed below. More specific descriptions of representative R&D requests in these program elements are included in Appendix I. Proposed projects may involve work in any activity of these program elements. However, they are not limited to the R&D topics provided in the appendix as long as they are relevant to overall programmatic objectives delineated in the Advanced Reactor, Fuel Cycle, and Energy Products Workshop for Universities web site.

If any proposed project involves use of the Advanced Test Reactor (ATR) for testing, experimentation, etc., all investigators for the project who would be working at the ATR must be U.S. citizens.

## 1. Advanced Fuel Cycle Initiative

**1.1 Spent Fuel Separations Technology** The separations technology development component of AFCI involves the development of advanced methods for the chemical partitioning of spent nuclear fuel into constituents that can be (1) readily disposed of in improved waste form, (2) recycled for transmutation and/or energy recovery in thermal and fast reactor systems, or (3) stored for future disposition (minor actinides, cesium and strontium). Such partitioning will be necessary for processing the output of current and future thermal spectrum reactors, and must incorporate the best available process technologies as well as state-of-the-art instrumentation for process monitoring/control and materials accountancy. There will also be special requirements for the processing of spent fuel arising from the operation of future Generation IV reactors that must be met in the future, utilizing advanced spent fuel treatment methods tailored to the unique fuel types of these reactor concepts. Proposed projects may involve R&D in the areas of advanced aqueous separations, pyrochemical processing, engineered product storage, and spent fuel treatment facility design/process technology development.

Appendix 1.1 describes specific current research needs that are relevant to this program element.

**1.2 Advanced Nuclear Fuel Development** This program element of the Advanced Fuel Cycle and Generation IV Initiatives is focused on conducting research and development activities for advanced fuels applicable to a variety of nuclear reactor systems. The fuel forms of interest are: (1) ultra-high-burnup fuels, mixed oxide fuels containing transuranic elements and inert matrix fuels containing transuranic elements for light-water reactors; (2) TRISO fuels with and without transuranic elements for high-temperature reactors; (3) advanced ceramic fuels (oxide, nitride, carbide) and metal fuels for liquid metal cooled fast reactors; and (4) composite fuels such as ceramics dispersed in metals (CERMET) and ceramics dispersed in ceramics (CERCER) for gas cooled or liquid metal cooled fast reactors. The fuels of interest for fast reactors and fast spectrum transmuters include fertile (high uranium content), low-fertile (low uranium content) and non-fertile (no uranium content) compositions in ceramic, metal, and composite fuels. The general research topics of interest cover wide-ranging areas of fuel modeling, fabrication process development, characterization methods, in-pile and out-of-pile testing, advanced instrumentation for in-pile testing, advanced fuel matrix and cladding material development.

If any proposed project involves use of the Advanced Test Reactor (ATR) for testing, experimentation, etc., all investigators for the project who would be working at the ATR must be U.S. citizens.

Appendix 1.2 describes specific current research needs that are relevant to this program element.

**1.3 Transmutation Science and Engineering Technologies** Transmutation science and engineering technologies provide critical R&D to support the AFCI transition fuel cycle, AFCI equilibrium fuel cycle, and Generation IV technologies, specifically in the areas of: (1) physics, (2) materials, (3) coolant technology, and (4) accelerator-driven systems (ADS). Transmutation is a process by which long-lived radioactive species, particularly actinides (but also certain fission products), are converted into short-lived nuclides by either fission or neutron capture. By changing the decay timescale from millennia to hundreds of years, radio-toxicity and

heat load challenges to the U.S. geologic repository fall into the realm of well-known engineering practices, and thus become easier to solve with better certainty of success. Transmutation science and engineering activities are focused in the areas of nuclear data and codes, coolants and corrosion, structural materials, and accelerator-based transmutation. Proposed projects may involve R&D in the areas of advanced corrosion resistant materials, modeling of corrosion kinetics, modeling of material behavior during irradiation, material irradiation performance, Monte Carlo physics code development, and safety parameter measurements.

Appendix 1.3 describes specific current research needs that are relevant to this program element.

**1.4 Advanced Fuel Cycle Systems Analysis** The role of advanced fuel cycle systems analysis is to link the objectives, analyses and technology developments of the Advanced Fuel Cycle Initiative with current operating nuclear plants and the Generation IV and Nuclear Hydrogen Initiatives by providing the models, tools, and analyses needed to define the best deployment options and to understand their benefits and impacts. Systems analyses of reactors and processes also will be useful for establishing needs for new technologies. Such studies typically involve cost analyses and comparisons and are ripe for innovative R&D in areas such as computer model development.

In the intermediate term, the top-level objective for systems analysis is to analyze spent fuel treatment and recycle options for current light water reactors to support a Secretarial recommendation on the technical need for a second repository after the end of CY 2007. High-level longer-term objectives for systems analysis include cost/benefit analyses of alternative Generation IV systems and their fuel cycles, with an eye to optimizing and downselecting the integrated reactor/fuel designs and developing their deployment strategies. In particular, deployment strategies need to consider trade-off options among economics, energy, environmental impacts, and nonproliferation benefits of integrated advanced reactor/fuel cycle systems, balanced by an understanding of their development costs and technology risks.

Appendix 1.4 describes specific current research needs that are relevant to this program element.

**1.5 Other AFCI Research** This category is provided to encourage innovative R&D in the general advanced fuel cycle area that may not be included in the AFCI program plan and that may not fall readily into the other categories listed. Research in innovative areas is expected to support the overall mission and objectives of the AFCI program, although reflecting ideas and concepts that have not been previously considered. The starting point for identifying what technologies are currently being investigated is the Fiscal Year 2003 *Report to Congress on Advanced Fuel Cycle Initiative: The Future Path for Advanced Spent Fuel Treatment and Transmutation Research* and the AFCI Comparison Reports for FY 2003 and later years. These are available at [www.nuclear.gov](http://www.nuclear.gov), under Public Information/Congressional Reports.

## **2. Generation IV Nuclear Energy Systems Initiative**

**2.1 Supercritical Water-Cooled Reactor** The SWCR has been selected as a Generation IV candidate system because it builds on proven current light water technology and offers the potential for considerably higher thermal efficiency. Over the next 3 years, the Generation IV R&D program for SCWR will focus on key feasibility issues for this concept and

address six critical issues identified in *A Technology Roadmap for Generation IV Nuclear Energy Systems*:

- Improve current models for analyzing the neutronics and thermal hydraulics of water-cooled systems at supercritical conditions and establish a baseline design for the SCWR core and reactor coolant system;
- Generate basic data on heat transfer, pressure drop and critical flow for supercritical water at SCWR prototypical conditions;
- Identify suitable safety systems and containment designs to cope with the consequences of major abnormal events;
- Evaluate the susceptibility of the SCWR to thermal-hydraulic and coupled thermal-hydraulic/neutronic instabilities;
- Develop a strategy for reactor control, including start-up and operational transients; and
- Evaluate the susceptibility of candidate core structural materials to corrosion and stress-corrosion cracking in supercritical water.

Appendix 2.1 describes specific current research needs that are relevant to this program element.

**2.2 Next Generation Nuclear Plant** The Next Generation Nuclear Plant (NGNP) is envisioned to be a high temperature reactor utilizing TRISO particle fuel in either a matrix or pebble bed configuration. The NGNP coolant is most likely either helium or possibly a molten fluoride salt. The NGNP project R&D needs in the areas of reactor and plant design and licensing include 1) further assessment and verification of the various available neutronic and thermal-hydraulic code capabilities, 2) integral and separate effects experiments to produce additional data to assess the thermal-hydraulic codes, 3) development of a credible air ingress analysis capability, 4) methods development for better modeling the NGNP balance of plant, 5) assessment of fuel cycles and core designs that take advantage of the “Deep Burn” capabilities and high power conversion efficiencies of gas-cooled reactors, 6) experimental assessment and mathematical modeling of pebble flow in the pebble bed version of the NGNP, and, 7) improved NGNP severe accident analysis modeling.

The NGNP project R&D needs in the area of materials research include 1) a better understanding of graphite irradiation induced swelling and shrinkage, 2) development of high temperature carbon/carbon ( $C_f/C$ ) or silicon-carbide/silicon-carbide ( $SiC_f/SiC$ ) control rod cladding and guide tubes materials, 3) development of materials and diffusion bonding techniques for compact high temperature intermediate heat exchangers (IHXs), 4) development of a better understanding of the high temperature materials interactions and potential degradation caused by low levels of impurities transported in the helium coolant, 5) additional mechanical property, weldment, stress rupture, and fatigue data, aging effects information, and further structural design methodology information for ASME codification of Alloy 617, Mod 9Cr-1Mo steel, and Hastelloy X, and, 6) research on alloying, materials processing, or coating techniques to improve the high temperature mechanical or environmental performance the NGNP metallic structural materials.



Appendix 2.2 describes specific current research needs that are relevant to this program element.

**2.3 Lead Alloy Liquid-Metal-Cooled Fast Reactor** Lead- Cooled Fast Reactor (LFR) activities are focused on the development of a small modular concept that would be suitable for deployment in remote locations and in developing countries – locations where transportation costs add to the cost of energy and where there is no physical infrastructure to support fuel handling and management. For that reason, the LFR program is directed toward meeting the following design objectives: small power output of 10 to 50 MWe; walk-away passive safety; a sealed core with a refueling cycle of 20 to 30 years to impart robust proliferation resistance; and a natural circulation primary system and autonomous load following to simplify plant construction and operation. Liquid metal-cooled reactors, and heavy metal-cooled reactors in particular, have characteristics that make them uniquely suited for meeting the design objectives.

These objectives raise several technical, deployment-related and institutional challenges. Technical challenges include identifying materials of construction and establishing a database on their performance to support licensing of an LFR; design of the core and internals to accomplish objectives for long core lifetime, passive safety, autonomous load following, and natural circulation; and engineering to address infrequent but necessary core changeout, in-service inspection and materials verification needs within a closed core, and energy conversion to appropriate energy products.

Appendix 2.3 describes specific current research needs that are relevant to this program element.

**2.4 Gas-Cooled Fast Reactor** The gas-cooled fast reactor (GFR) was chosen as one of the Generation IV nuclear reactor systems to be developed based on its excellent potential for sustainability through reduction of the volume and radiotoxicity of both its own fuel and other spent nuclear fuel, and for extending/utilizing uranium resources orders of magnitude beyond what the current open fuel cycle can realize. In addition, energy conversion at high thermal efficiency is possible with the current designs being considered, thus increasing the economic benefit of the GFR. The reference design uses a direct-cycle helium turbine for electricity (42% efficiency at 850°C), and process heat for thermochemical production of hydrogen.

An alternate design is also a helium-cooled system, but utilizes an indirect Brayton cycle for power conversion. Research and design of a secondary system utilizing supercritical CO<sub>2</sub> (S-CO<sub>2</sub>) at 550°C and 20 MPa is an area of high interest. The principal challenge of any of these designs is system performance under accident conditions. Research on approaches to achieving passive safety while maintaining high power densities that favor economics is desired. Research on heat removal approaches under extreme accident situations is also of interest.

Appendix 2.4 describes specific current research needs that are relevant to this program element.

**2.5 Design and Evaluation Methods Development** This program element addresses the need for validated design and safety analysis methods and for methodologies to evaluate system performance against Generation IV goals. Design analysis of each Generation IV system requires a validated set of modeling approaches, computer codes, and databases to simulate neutronic, thermal, fluid flow, and mechanical/structural behavior in steady-state and transient conditions. Examples are the computer codes and databases used for reactor physics

and fuel depletion analysis, thermal-hydraulic and thermo-structural design analysis, and simulation of postulated accident sequences. Advances are targeted in each area to help reduce uncertainties in predicted system behavior and contribute to developing optimized Generation IV system designs.

A need has also been identified in the Generation IV Technology Roadmap to advance methodologies for evaluating overall system performance against the Generation IV goals of sustainability, economics, safety, reliability, proliferation resistance, and physical protection. Compared to capabilities previously employed for such evaluations, targeted advances include increased quantification of performance measures, better characterization of uncertainty in evaluated performance, representation of unique features of Generation IV systems, and a more comprehensive consideration of important factors affecting performance. Application of these methodologies will help guide the R&D on the systems and provide a basis for judging the success of the R&D as it progresses, as well as for the selection of preferred systems and system design options.

Appendix 2.5 describes specific current research needs that are relevant to this program element.

**2.6 Crosscutting Materials Development for Advanced Reactors** This program element involves the R&D required to study, quantify, and in some cases, develop materials with necessary properties for the Gen IV advanced reactor systems. For the range of service conditions expected in Gen IV systems, including possible accident scenarios, sufficient data must be developed to demonstrate that the candidate materials meet the following design objectives: (1) acceptable dimensional stability including void swelling, thermal creep, irradiation creep, stress relaxation, and growth; (2) acceptable strength, ductility, and toughness; (3) acceptable resistance to creep rupture, fatigue cracking, creep-fatigue interactions, and helium embrittlement; and (4) acceptable chemical compatibility and corrosion resistance (including stress corrosion cracking and irradiation-assisted stress corrosion cracking) in the presence of coolants and process fluids. Additionally, it will be necessary to develop validated models of microstructure-property relationships to enable predictions of long-term materials behavior to be made with confidence and to develop high-temperature materials design methodology for materials, use, codification, and regulatory acceptance.

Appendix 2.6 describes specific current research needs that are relevant to this program element.

**2.7 Energy Conversion** Generation IV Energy Conversion work focuses development on more efficient or lower cost electrical conversion technologies for the outlet temperature ranges of interest to Generation IV reactors. Most of the Generation IV reactor concepts will have output temperatures in the range 550 to 700 C. The VHTR is being developed to have output temperatures of ~1000 C. Brayton cycles using inert or other gas working fluids are promising technologies for these temperature ranges, and advanced cycles can be developed in the time frame of interest for Generation IV reactors. Near-term R&D includes research on supercritical CO<sub>2</sub> cycle systems and turbomachinery design, assessment of high temperature Brayton cycle efficiency and costs, and assessment of NGNP power conversion technology options. Primary focus is being placed on the supercritical CO<sub>2</sub> cycle. Energy Conversion activities for the high temperature Brayton systems focus on thermodynamic analyses to assess a range of options for improvements in cycle efficiency or conversion system cost.

Energy Conversion activities also include an analysis of baseline options for power conversion systems for the NGNP. The investigation of advanced power conversion options for Generation IV reactors will include scaled experiments to provide a validated technology basis for next generation engineering decisions. Initial demonstrations will involve laboratory scale experiments for components and key technologies to validate viability and performance assessments. For selected technologies, pilot plant demonstrations to assess engineering approach and performance will be performed.

Appendix 2.7 describes specific current research needs that are relevant to this program element.

**2.8 Other Generation IV Research** This category includes innovative concepts that may not be included in the Generation IV program plan. The Generation IV Nuclear Energy Systems Initiative has solicited and evaluated innovative reactors and energy systems, as documented in *A Technology Roadmap for Generation IV Nuclear Energy Systems*. The Roadmap's conclusions and recommendations are reflected in the Generation IV program as currently formulated, but further innovation is of interest. Applications in the category of Innovative concepts may offer new ideas and concepts that have not been considered before. Research in innovative areas is expected to support the overall mission and objectives of the Generation IV program. Areas of interest include fuels, materials, reactors, components, safety concepts, or other concepts that make nuclear energy safer, more economic, more sustainable, more proliferation-resistant, or more resistant to terrorist attack.

### 3. Nuclear Hydrogen Initiative

As part of the DOE Hydrogen Program, all hydrogen-related applications proposing experiments that handle hydrogen must include a preliminary safety plan, and all funded projects must complete a more detailed safety plan as part of the project within 60 days after award. This requirement is further defined in a Safety Requirements Document at [http://www.eere.energy.gov/hydrogenandfuelcells/pdfs/safety\\_guidance.pdf](http://www.eere.energy.gov/hydrogenandfuelcells/pdfs/safety_guidance.pdf)

**3.1 Thermochemical Cycles** DOE is investigating the use of thermochemical cycles for hydrogen production using high temperature advanced nuclear reactors. Thermochemical cycles involve a series of chemical reactions that produce hydrogen from water at lower temperatures than direct thermal dissociation of water. High temperature advanced reactors will provide the heat for the endothermic chemical reactions. This task area will focus on the development of thermochemical cycles suitable for coupling to a high temperature nuclear reactor. Analytic and lab scale experimental studies will be performed for the sulfur-iodine, hybrid sulfur and calcium bromine cycles to evaluate cycle performance and viability for use with nuclear energy. Analytic studies will also investigate several promising alternative cycles that may have potential for use with nuclear reactors, and lab scale experimental work will be initiated where appropriate. Flowsheet analyses will be performed to identify promising approaches, and lab scale experiments will confirm technical feasibility and performance potential. For the selected processes, engineering scale systems will be needed to demonstrate economically viable hydrogen production using nuclear heat.

Appendix 3.1 describes specific current research needs that are relevant to this program element.

**3.2 High Temperature electrolysis** This element of the Nuclear Hydrogen Initiative focuses on developing components and overall designs for splitting steam into hydrogen and oxygen using high-temperature solid-oxide electrolyzer cells (SOECs). The technology is

derived from the materials and configurations now used in solid oxide fuel cells (SOFCs) in fossil-fired applications. At the 750-850 °C operating temperatures of SOECs, about 30 percent of the energy for electrolysis is supplied thermally, increasing the overall efficiency of the process to about 45 percent. The high-temperature electrolysis (HTE) project has conducted “button cell” experiments to characterize the performance of the solid oxide electrolyte and is now beginning small stack experiments using five to ten 100 cm<sup>2</sup> cells in series to investigate the thermal and electrical performance of both the electrolyte and the interconnection plates. Some of the stack experiments will be of long duration to identify and understand mechanisms for cell degradation due to corrosion, creep and material transport in high temperature operation.

In addition, the project is developing conceptual designs for the series of experiments needed to demonstrate the concept on a commercial scale when attached to a 600-MWth VHTR. Besides the cells themselves, this design activity is determining requirements for electrical power control, steam-hydrogen separations and hydrogen and oxygen cooling. Finally, the project is investigating methods for reducing the overall costs of hydrogen production through HTE.

Appendix 3.2 describes specific current research needs that are relevant to this program element.

**3.3 Reactor-Hydrogen Production Process Interface** This program element includes the development of technologies to couple new hydrogen production systems to an advanced high-temperature nuclear reactor. This effort introduces new considerations and requirements into the design of heat transfer methods and nuclear hydrogen production. Both high-temperature electrolysis and thermochemical systems are planned to be co-located with the nuclear heat source. The interface between the reactor and hydrogen production system involves potentially long heat transfer paths at elevated temperatures, heat exchangers that are subject to both elevated temperature and corrosive chemical environments, new safety and regulatory issues, and supporting systems for chemical processes, and H<sub>2</sub> and O<sub>2</sub> management. Although some of these issues will be common to any nuclear hydrogen plant, many will depend on the specific hydrogen production process selected.

Appendix 3.3 describes specific current research needs that are relevant to this program element.

**3.4 Other Nuclear Hydrogen Production Research** This category is provided to encourage innovative R&D in the nuclear hydrogen production area that may not be included in the Nuclear Hydrogen R&D plan and that may not fall readily into the other categories listed. The Nuclear Hydrogen R&D Plan describes the activities that will be conducted under the Nuclear Hydrogen Initiative. The program is focused on developing technologies for demonstration with a nuclear reactor by 2017, but this development could be significantly augmented by alternative, innovative approaches to nuclear-assisted hydrogen production. Research in innovative areas is expected to support the overall mission and objectives of the NHI program. Applications in this category may include, but are not limited to, alternative hydrogen production R&D on processes that are not specifically excluded from the Nuclear Hydrogen Initiative as discussed in the Nuclear Hydrogen R&D Plan. As such, R&D topics being pursued by other components of the DOE Hydrogen Program, such as reforming of biomass and steam-methane reforming, are excluded from this solicitation.

**This announcement is intended only for applications from U.S. universities.**

Each application should involve only one topic of one program element. A university may submit more than one application, but separate applications must be used for each topic of each program element.

## **II. Award Information.**

### **1. Type of Award Instrument.**

- DOE anticipates awarding Cooperative Agreements under this Program Announcement. A special award condition describing the Government's substantial involvement in the cooperative agreement is located in Section VI.2.

### **2. Estimated Funding.**

- Approximately \$3,700,000 in FY 2004 funding and similar amounts in FY 2005 and FY 2006 is expected to be available for new awards under this announcement.

### **3. Maximum and Minimum Award Size.**

- There are no maximum or minimum award amounts.

### **4. Expected Number of Awards.**

- No estimates on the number of awards have been made.

### **5. Anticipated Award Size.**

- The average award size for this program is anticipated to be \$100,000 to \$300,000 per year.

### **6. Period of Performance.**

- DOE anticipates making awards that will run for up to 3 years conditional on the availability of appropriated funds and contractor performance.

### **III. Eligibility Information.**

#### **1. Eligible Applicants.**

- Applicant eligibility is restricted to U.S. colleges and universities. Any collaborators to be funded under this announcement through the lead universities or colleges may be other U.S. colleges or universities, DOE national laboratories, or industrial organizations. At least 75 percent of the requested funding must go to universities unless an adequate justification for a larger portion going to non-universities is provided. Letters of support from collaborators should be included in the application.
- If any proposed project involves use of the Advanced Test Reactor (ATR) for testing, Experimentation, etc., all investigators for the project who would be working at the ATR must be U.S. citizens.

#### **2. Cost Sharing or Matching**

- Cost sharing/matching is not required, but is strongly encouraged if non-university participants are included.

### **IV. Application and Submission Information.**

#### **1. Address to Request Application Package.**

- This announcement and its appendix includes all the information needed to complete an application.
- Application forms and formats are available at Procurement Services Division's Internet home page at <http://www.id.doe.gov/doeid/psd/proc-div.html>.

#### **2. Content and Form of Application Submission.**

##### **A. DUNS Number.**

All applicants, except individuals who would personally receive an award under this announcement apart from any business or non-profit organization they may operate, must include a Dun and Bradstreet (D&B) Data Universal Numbering System (DUNS) number in their application. For the purpose of this requirement, the applicant is the entity that meets the eligibility criteria and has the legal authority to apply for an award. For example, a consortium formed to apply for an award must obtain a DUNS number for that consortium. For assistance in obtaining a DUNS number at no cost to you, call the DUNS Number request line at 1-866-705-5711. Be prepared to provide the following information: 1) Organization name; 2) Address; 3) Local telephone number; 4) Name of the CEO/business owner; 5) Legal structure of the business (corporation, partnership, etc.); 6) Year the organization started; 7) Primary line of business; 8) Total number of employees (full and part time). If you

do not already have a DUNS number, you should obtain one as soon as you decide to submit an application

**B. Letter of Intent.**

- Letters of Intent are not required.

**C. Pre-application**

- Pre-applications are not required.

**D. Application.**

- Applicants must include the following files in their E-Application (See Section IV.6. "Other Submission Requirements" for instructions on how to submit your E-Application):

**i. Application File.**

Applicants must complete a SF 424 application form. Save this form as an Adobe Portable Document Format (PDF) file, named "Application." The SF 424 application form may be found on PSD's Internet web site at <http://www.id.doe.gov/doi/psd/proc-div.html>.

**ii. Budget Files.**

- Budget File. Applicants must complete a DOE F 4620.1 for each year of support requested and a cumulative budget for the total project period. This form will be made available under this solicitation as a separate file as an excel worksheet. You may request funds under any of the categories listed as long as the item and amount are necessary to perform the proposed work and are not precluded by the cost principles or program funding restrictions (see Section IV.5).
- Budget Justification File. In addition to the DOE 4620.1, provide justification for the proposed direct labor, travel, consultants, large subawards, large or unique "other direct costs," equipment, etc., and the basis for the cost estimate. Any required foreign travel must be specifically identified and justified. For subawards, identify organization name, description of the scope of work, name of the project leader, and estimated total costs. Subawards in excess of \$100,000 or more will need the same cost breakdown and justification detail as the applicant's level of detail. Provide an explanation of the source, nature, amount and availability of any proposed cost sharing. The contracting officer may request for additional cost justification or support for a particular subaward, if your application is selected.

### **iii. Project Summary/Abstract.**

The project summary/abstract must contain a summary of the proposed activity using the format provided in Attachment A. It should be a self-contained document that identifies the name of the applicant, the program and program element the project supports, the project title, the principal investigator, any collaborators, the abstract, and a summary budget table. The abstract (maximum of two paragraphs) must be suitable for public release and should include the objectives of the project, its scope and how it supports the program element, the methods to be employed, and the potential impact of the project (i.e., benefits, outcomes). It should be informative to other persons working in the same or related fields and, insofar as possible, understandable to a scientifically or technically literate lay reader. This document must not include any proprietary or sensitive business information as the Department may make it available to the public. The project summary must not exceed 1 page when printed using standard 8.5" by 11" paper with 1" margins (top, bottom, left and right) with font not smaller than 11 point. Save this information in an MS Word file, named "Project Summary."

### **iv. Project Narrative File.**

The project narrative file must be formatted to separately address each of the sections listed below. Each section must not exceed the specified page limitation, if any, when printed using standard 8.5" by 11" paper with 1 inch margins (top, bottom, left, and right). The type must be legible and not smaller than 11 point. Evaluators will review only the number of pages specified.

Unnecessarily elaborate applications are not desired. Elaborate artwork, graphics and pictures will increase the document file size. If the project narrative file size is over 5MB, we request that you use a "Zip" file compression software, such as WinZip software, to reduce the time needed to download the file. Save all the project component information in a single file, named "Project Narrative."

- Project Narrative. This section should provide a clear description of the work to be undertaken and how you plan to accomplish it. It must be formatted to address each of the merit review criterion and sub-criterion listed in Section V.B. Provide sufficient information so that the reviewers will be able to evaluate the application in accordance with these merit review criteria. **DOE WILL EVALUATE AND CONSIDER ONLY THOSE APPLICATIONS THAT ADDRESS SEPARATELY EACH OF THE MERIT REVIEW CRITERION AND SUB-CRITERION.**

The project narrative section must not exceed 5 pages. Graphics and visual material, including charts, graphs, maps, photographs and other pictorial presentations, will be counted in the page limitation for this section.



- *Special instructions for applications that contain graphics and visual material.* All graphics and visual material should be referenced in the project narrative text, converted to pdf files (such as Adobe Acrobat Portable Document Files), and included as a separate attachment, named "Graphics Attachment." (See Section IV.2.D.iv.)
- Relevance and Justification. This section should explain the relevance of the effort to the objectives in the funding opportunity announcement. The justification for the proposed project should include a clear statement of the importance of the project in terms of the utility of the outcomes to the relevant program element. This section must not exceed 1 page.
- Roles of Participants. For multi-organizational or multi-investigator projects, describe the roles and the work to be performed by each participant/investigator including any business agreements between the applicant and participants, and how the various efforts will be integrated and managed. This section must not exceed 1 page.
- Project Activities and Schedule. This section should identify the activities/tasks to be performed, project milestones, and the expected dates for the release of deliverables, by project year (starting with October 2005) and how the project milestones support the program and program element milestones and schedule. This section should identify any decision points and go/no-go decision criteria. Successful applicants must use this project schedule and these milestones to report progress. This section must not exceed 2 pages
- Evaluation Phase. This section must include a plan and metrics to be used to assess the success of the project. This section must not exceed 1 page.
- Facilities and Other Resources. Describe the facilities (e.g., office, laboratory, animal, computer, etc.) to be used at each performance site listed and, if appropriate, indicate their capacities, pertinent capabilities, relative proximity and extent of availability to the project. Describe only those resources that are directly applicable to the proposed work. Provide any information describing the other resources available to the project such as machine or electronic shops. This section must not exceed 1 page.
- Equipment. List important items of equipment already available for this project and, if appropriate, note the location and pertinent capabilities of each. If you are proposing to acquire equipment, describe comparable equipment, if any, already at your organization and explain why it cannot be used. This section must not exceed 1 page.
- Bibliography and References, if applicable. Provide a bibliography for any references cited in the Project Narrative section. This section must include only bibliographic citations.

**v. Certifications/Assurances/Representations.**

Applicants must complete the DOE certification/assurance/representation information. Save this information in a single MS Word file named "Certifications&Assurances". [Click here for form](#)

**vi. Attachment Files.**

Applicants must submit the following additional files with their applications.

- Biographical Sketch.

Provide a biographical sketch for the project director/principal investigator, co-project directors/principal investigators. Save this information in a single file, named "Bio Attachment." The biographical information must not exceed 2 pages for each person when printed on 8.5" by 11" paper with 1 inch margins (top, bottom, left, and right) with font not smaller than 11 point and must include:

- Education. Undergraduate, graduate and postdoctoral training, provide institution, major/area, degree and year.
- Positions. Beginning with the current position, list in chronological order professional/academic positions with a brief description.
- Publications. A list of up to 5 publications most closely related to the proposed project. For each publication, identify the names of all authors (in the same sequence in which they appear in the publication), the article title, book or journal title, volume number, page numbers, year of publication, and website address if available electronically.
- Patents, copyrights and software systems developed may be provided in addition to or substituted for publications.
- Synergistic Activities. List no more than 5 professional and scholarly activities related to the effort proposed.

- Graphics and Visual Material.

Applicants must submit project graphics and visual material in a separate attachment, named "Graphics Attachment." See Project Narrative, paragraph 3, "Special instructions for applications that contain graphics and visual material."

### 3. Submission Dates and Times.

#### A. Application due date:

- Applications and amendments to applications must be received by **July 16, 2004**, not later than 5:00 PM Mountain Daylight Time. You are encouraged to transmit your application well before the deadline. APPLICATIONS, INCLUDING ALL APPLICATION FILES, RECEIVED AFTER THE DEADLINE, AS DEMONSTRATED BY THE IIPS DATE/TIME STAMP, WILL NOT BE REVIEWED OR CONSIDERED FOR AWARD.

#### B. Submissions from Successful Applicants.

- Successful applicants will be notified to submit additional information such as additional cost sheet, Certifications, RTS-2 information sheet etc.

### 4. Intergovernmental Review.

- This program is not subject to Executive Order 12372 - Intergovernmental Review of Federal Programs.

### 5. Funding Restrictions.

- **Cost Principles.** Costs must be allowable in accordance with the applicable cost principles referenced in 10 CFR part 600.
- **Pre-Award Costs.** Recipients if selected may charge to an award resulting from this announcement pre-award costs that were incurred within the ninety (90) calendar day period immediately preceding the effective date of the award, if the costs are necessary for the conduct of the project activities and are otherwise allowable in accordance with the applicable cost principles and the terms and conditions of the award. Recipients must obtain the prior approval of the contracting officer for any pre-award costs that are for periods greater than this 90 day calendar period.

Pre-award costs are incurred at the applicant's risk. DOE is under no obligation to reimburse such costs if for any reason the applicant does not receive an award or if the award is made for a lesser amount than the applicant expected.

- **Foreign Travel.** Cost of foreign travel is allowable under an award made pursuant to this announcement. All foreign travels cost shall be included as a separate line item in the cost proposal.

### 6. Other Submission Requirements

- **Electronic Submission.** Applications must be submitted through the DOE Industry Interactive Procurement System (IIPS) at <http://e-center.doe.gov>. Instructions on

how to submit an application or an application amendment and how to register, submit questions, and view questions and answers are located on the web site at <http://e-center.doe.gov>. Click on the Help button. Click on the Frequently Asked Questions button.

Prepare all the required files in accordance with the instructions in this announcement prior to starting the transmission process. Submit the entire application package in one IIPS session (i.e., do not logoff before all the files are submitted.)

When you are ready to submit your application, go to <http://e-center.doe.gov> and complete the IIPS cover page. Enter the project title and the principal investigator/project director, if any, in the "Subject" block. Then attach each file in the corresponding block in accordance with the IIPS guidance. Follow the instructions for submitting the application.

If you have any problems accessing information or submitting your application, contact the Help Desk at 1 800-683-0751 and select option 1, or send an email to [HelpDesk@pr.doe.gov](mailto:HelpDesk@pr.doe.gov). ONLY APPLICATIONS SUBMITTED THROUGH IIPS WILL BE CONSIDERED FOR AWARD.

- **Electronic Signature.** Applications submitted through IIPS constitute submission of electronically signed applications. The name of the authorized organizational representative (i.e., the administrative official, who, on behalf of the proposing organization, is authorized to make certifications and assurances or to commit the applicant to the conduct of the project) must be typed in the signature block on the form to be accepted as an electronic signature. Do not submit a scanned copy of the signed document.
- **IIPS Registration.** In order to submit an application, you must be authorized by the applicant (i.e., institution or business entity) to submit an application on its behalf and you must register in IIPS. You are encouraged to register as soon as possible. You only have to register once to apply for any DOE award. To register, go to <http://e-center.gov> and follow the registration instructions.
- In addition to the electronic submittal to the IIPS system one original hard copy of the proposal must be submitted to:

Procurement Services Division  
U. S. DOE, Idaho Operations Office  
Attention: Seb Klein [DE-PS07-01ID14554]  
1955 Fremont Avenue  
Idaho Falls, ID 83401-1221

## V. Application Review Information

### 1. Criteria.

#### A. Initial Review Criteria

- Prior to a comprehensive merit evaluation, DOE will perform an initial review to determine that (1) the applicant is eligible for an award; (2) the information required by the announcement has been submitted; (3) all mandatory requirements are satisfied; and (4) the proposed project is responsive to the objectives of the funding opportunity announcement.

## **B. Merit Review Criteria.**

- The following evaluation criteria and the associated weighting factors (in parentheses) apply to the objective merit review:
  1. Technical quality of the proposed work (40%)
    - a. Contribution to the state of knowledge in the relevant program element and applicable scope;
    - b. Completeness and clarity of the technical application;
    - c. Appropriateness/adequacy of the proposed methodology or approach;
  2. Extent to which proposed work will meet the requirements of the relevant program element and scope of work specified in Section I; and if successful would significantly advance the state of the art in that program (25%);
  3. Capabilities and qualifications of principal investigator/project manager and key personnel; adequacy of resources and facilities applied by participating organization (10%);
  4. Reasonableness of the proposed project cost and schedule (25%).

## **C. Application Review Process**

- **Merit Review.** An objective merit – peer review will be performed to evaluate the technical and/or scientific quality, merit, and cost aspects of the applications, exclusive of programmatic and policy factors. This peer review will be in accordance with the evaluation criteria stated above. Each application will be evaluated on its own merit and independently of any other applications. For this purpose, three or more professionally and technically qualified persons will be selected in such a manner as to assure the highest degree of independence and objectivity. The reviewers may include any mix of federal and non-federal (national laboratory, university, and other) experts, except for those persons involved in the relevance review or approving/disapproving the applications. Reviewers must comply with the requirements for avoiding conflict of interest as stated in 10 CFR 600.14. (Universities that have submitted applications in the same program element are excluded.)
- **Relevance Review.** Following the merit reviews, a programmatic relevance review will be performed by DOE program directors and managers with input from national laboratory program managers that are not part of the merit review (National Technical Directors and System Integration Managers). The relevance reviews will be performed on those applications judged to be of high technical merit. The applications will be evaluated with respect to programmatic and policy factors, including relevance of the proposed work to the program objectives, balance among

program elements to be supported, availability of funds, and conformance to DOE policy and programmatic objectives.

- **Management Review:** Following the relevance review, DOE management will make the final review and selection of awards. The Office of Nuclear Energy, Science and Technology's Deputy Director for Technology will be the source selection official.

#### **D. Discussions and Award.**

- The Government may enter into discussions with a selected applicant for any reason deemed necessary, including but not limited to: (1) the budget is not appropriate or reasonable for the requirement; (2) only a portion of the application is selected for award; (3) the Government needs additional information to determine that the recipient is capable of complying with the requirements in 10 CFR 600; and/or (4) special terms and conditions are required. Failure to resolve satisfactorily the issues identified by the Government will preclude award to the applicant.

#### **2. Anticipated Announcement and Award Dates.**

- DOE anticipates notifying applicants selected for award by **September 2004** and making awards by **October 2004**.

### **VI. Award Administration Information.**

#### **1. Award Notices.**

##### **A. Notice of Selection.**

- DOE will notify applicants selected for award. This notice of selection is not an authorization to begin performance. (See Section IV.5 with respect to the allowability of pre-award costs.)
- Organizations whose applications have not been selected will be advised as promptly as possible.

##### **B. Notice of Award.**

- A Notice of Financial Assistance Award issued by the contracting office is the authorizing award document. It includes, either as an attachment or by reference: 1. a budget, that indicates the amounts, by categories of expenses, on which the agency has based its support; 2. the application; 3. applicable program regulations, if any; 4. special terms and conditions; 5. DOE assistance regulations at 10 CFR 600, or, for Federal Demonstration Partnership (FDP) institutions, the FDP terms and conditions; and 6. a reporting checklist, which identifies the reporting requirements.

## **2. Administrative and National Policy Requirements.**

### **A. Administrative Requirements.**

The administrative requirements and national policy requirements (e.g., "generally applicable requirements") for DOE grants and cooperative agreements are contained in 10 CFR Part 600, except for grants made to Federal Demonstration Partnership (FDP) institutions. The FDP terms and conditions and DOE FDP agency specific terms and conditions are located on the National Science Foundation web site at [http://www.nsf.gov/home/grants/grants\\_fdp.htm](http://www.nsf.gov/home/grants/grants_fdp.htm). "Generally applicable requirements" are defined in 10 CFR 600.12

### **B. Special Terms and Conditions.**

#### **Lobbying**

##### **Lobbying Restrictions.**

The recipient agrees that none of the funds obligated on this award shall be expended, directly or indirectly, to influence congressional action on any legislation or appropriation matters pending before Congress, other than to communicate to Members of Congress as described in 18 U.S.C. 1913. This restriction is in addition to those prescribed elsewhere in statute and regulation.

#### **Buy American Act.**

##### **NOTICE REGARDING THE PURCHASE OF AMERICAN-MADE EQUIPMENT AND PRODUCTS -- SENSE OF CONGRESS**

It is the sense of the Congress that, to the greatest extent practicable, all equipment and products purchased with funds made available under this award should be American-made.

#### **Reporting.**

Failure to comply with the reporting requirements contained in this award will be considered a material noncompliance with the terms of the award. Noncompliance may result in withholding of future payments, suspension or termination of the current award, and withholding of future awards. A willful failure to perform, a history of failure to perform, or of unsatisfactory performance of this and/or other financial assistance awards, may also result in a debarment action to preclude future awards by Federal agencies.

#### **Environmental, Safety, and Health.**

The recipient must comply with applicable federal, state, and local environmental, safety, and health laws and regulations for work performed under this award.

#### **Notice Regarding Unallowable Costs and Lobbying Activities.**

The recipient should carefully review the allowable cost and other provisions applicable to expenditures under this award. If funds are spent for purposes or in amounts inconsistent with the allowable cost or any other provisions governing expenditures, DOE may pursue a number of remedies, including in appropriate

circumstances, recovery of such funds, termination of the award, suspension or debarment, and criminal prosecution for false statements.

Particular care should be taken to comply with all statutes and regulations prohibiting the expenditure of funds for lobbying and related activities. Financial assistance awards may be used to describe and promote the understanding of scientific and technical aspects of specific energy technologies, but not to encourage or support political activities such as the collection and dissemination of information related to potential, planned, or pending legislation.

#### **Statement of Substantial Involvement.**

DOE anticipates having substantial involvement during the project period, through technical assistance, advice, intervention, integration with other awardees performing related activities, and technology transfer activities. The recipient's responsibilities are listed in paragraph A and the DOE's responsibilities are listed in paragraph B.

- A. The recipient is responsible for:
  - 1. Performing the activities supported by this award, including providing the required personnel, facilities, equipment, supplies and services.
  - 2. Defining approaches and plans, submitting the plans to DOE for review, and incorporating DOE comments.
  - 3. Managing and conducting the project activities, including coordinating with DOE and DOE contractors on activities related to the project.
  - 4. Attending semi-annual program review meetings and reporting project status.
  - 5. Submitting technical reports to the DOE Program Director and incorporating DOE comments and:
  - 6. Presenting the project's results at appropriate technical conferences or meetings as directed by the DOE Program Director (number of conferences/meetings will not exceed 2 per year, not counting program review meetings.)
- B. DOE is responsible for:
  - 1. Reviewing in a timely manner project plans, including technology transfer plans, and redirecting the work effort if the plans do not address critical programmatic issues.
  - 2. Conducting semi-annual program review meetings to ensure adequate progress and that the work accomplishes the program and project objectives. Redirecting work or shifting work emphasis, if needed.
  - 3. Promoting and facilitating technology transfer activities, including disseminating program results through presentations and publications



4. Serving as scientific/technical liaison between awardees and other program or industry staff.

### 3. Reporting

- **Reporting Requirements.** Reporting requirements are identified on the Federal Assistance Reporting Checklist, DOE F 4600.2, attached to the award agreement. See <http://www.id.doe.gov/doeid/psd/proc-div.html> for the proposed Checklist for this program.

- **Special Reporting Requirements for Cooperative Agreements.**

The special reporting requirements for cooperative agreements will be incorporated in cooperative agreements awarded under this announcement. Each project will have specific reporting requirements

- **Procurement Services Division's Report Tracking System-2 (RTS-2) Database**
  - Procurement Services Division uses a database (RTS-2) to track report deliverables. Each new financial assistance award is entered into RTS-2. The system is programmed to send automatic email reminders approximately three weeks before a report is due. The reminder notice identifies which report is due, the time period that the report should cover, and the report due date.
  - If a report is not received by the report due date, the report is "late." Once a report is "late," it is always designated by the system as "late." A "delinquent" report is a report that has not yet been received by Procurement Services Division. A "delinquent" report is always late. However, a "late" report may not be delinquent (i.e., not yet received).
  - The system automatically sends two delinquent reminder notices. The first delinquent notice is sent approximately 10 days after the report was due. The second delinquent notice is sent approximately 30 days after the report was due.
  - Reports submitted to Procurement Services Division should be sent electronically to [psdrept@id.doe.gov](mailto:psdrept@id.doe.gov). The "report received" date is the date that Procurement Services Division receives the report. The system sends an email acknowledgment of receipt when a report is logged into RTS-2.

## II. Agency Contacts

- **FOR FURTHER INFORMATION OR QUESTIONS AND ANSWERS CONTACT:** Questions shall be submitted to Seb Klein, contract specialist, by facsimile at 208-526-5548, e-mail: [kleinsm@id.doe.gov](mailto:kleinsm@id.doe.gov), or by telephone at (208) 526-1901 no later than June 26, 2004. Questions and answers to the questions will be posted to the Industry Interactive Procurement System (IIPS) Website by July 1, 2004 as an amendment to this solicitation.

## **VII. Other Information.**

### **1. Modifications.**

Notices of any modifications to this announcement will be posted on the DOE Industry Interactive Procurement System (IIPS).

If you register in IIPS, you may join this solicitation mailing list to receive an email when a modification or an announcement message is posted. To view modifications and announcement messages, locate the announcement on IIPS and click on the yellow folder next to the announcement number or follow the directions for "Locate Solicitation."

### **2. Government Right to Reject or Negotiate**

DOE reserves the right, without qualification, to reject any or all applications received in response to this announcement and to select any application, in whole or in part, as a basis for negotiation and/or award.

### **3. Commitment of Public Funds**

The Contracting Officer is the only individual who can make awards or commit the Government to the expenditure of public funds. A commitment by other than the Contracting Officer, either explicit or implied, is invalid.

### **4. Proprietary Application Information**

No proprietary data will be allowed

### **5. Evaluation by Non-Federal Reviewers**

In conducting the merit review evaluation, the Government plans to use qualified non-Federal personnel (e.g., DOE management and operating contractors, or other scientific/technical experts) as reviewers or advisors. The applicant, by submitting its application, consents to the use of non-Federal reviewers. Non-Federal reviewers will be required to sign a Conflict-of-Interest/Non-Disclosure Certificate prior to reviewing any application.

### **6. Intellectual Property Developed under this Program**

Patent Rights. The government will have certain statutory rights in an invention that is conceived or first actually reduced to practice under a DOE award. 42 U.S.C. 5908 provides that title to such inventions vests in the United States, except where 35 U.S.C. 202 provides otherwise for nonprofit organizations or small business firms. However, the Secretary of Energy may waive all or any part of the rights of the United States subject to certain conditions

Rights in Technical Data. Normally, the government has unlimited rights in technical data created under a DOE agreement. Delivery or third party licensing of proprietary software or data developed solely at private expense will not normally be required except as specifically negotiated in a particular agreement to satisfy DOE's own needs or to insure the commercialization of technology developed under a DOE agreement.

Intellectual Property Provisions. The standard DOE financial assistance intellectual property provisions applicable to the various types of recipients are located at [www.gc.doe.gov/gcmain.html](http://www.gc.doe.gov/gcmain.html). Click here for provisions.

## ATTACHMENT A

### SUMMARY/ABSTRACT PAGE FORMAT

A summary page (one page limit) should be provided in the following format using no smaller than an 11-point Arial or equivalent font type print.

**Applicant:**

**Program and Program Element:**

**Project Title:**

**Principle Investigator:** (Include name, organization, mailing address, phone number, fax number, e-mail, and congressional district.)

**Collaborators:** (Include name, organization, mailing address, phone number, fax number, e-mail, and congressional district.)

**Abstract:** (Nonproprietary summary of proposed project, including project benefits suitable for public release (maximum of two paragraphs))

**Budget Table:**

Budget	Total Funding <sup>1</sup>	DOE Funding
Total Project		
Year 1		
Year 2		
Year 3...		

<sup>1</sup> Includes DOE and any cost share funding

## APPENDIX 1

### Detailed Scope of Work in the Program Elements

Proposed projects may involve work in any activity of these program elements. Some examples of specific current research needs of interest to each program element are listed below. However, proposals are encouraged beyond the listed R&D topics so long as they are relevant to the goals of the Advanced Fuel Cycle Initiative, the Generation IV Nuclear Energy Systems Initiative, or the Nuclear Hydrogen Initiative.

#### 1. Advanced Fuel Cycle Initiative

##### 1.1 Spent Fuel Separations Technology

The listing of some R&D needs below is organized according to programmatic activity categories.

##### Advanced Aqueous Separations

- Evaluate the chemistry of plutonium extraction in the UREX+1 (UREX/TRUEX or equivalent) and UREX+2 (co-decontamination) processes.
- Develop a conceptual hybrid aqueous/non-aqueous process for the treatment of LWR spent fuel that minimizes process complexity and leads to reduced operating costs.
- Develop a process for the conversion of technetium strip solution from the UREX+1 and UREX+2 processes to metallic form for incorporation in a metallic waste form.
- Model and design organic extractants having acceptable radiation stability that can be used in a one-step separation of:
  - Americium and curium from lanthanide fission products with a decontamination factor  $>10^4$ .
  - Americium from curium, after lanthanide removal, with a decontamination factor  $>10^4$
- Synthesize stable advanced extractant solvent molecules with high specificity for minor actinides (Np, Am, Cm).

##### Pyrochemical Processing

- Develop corrosion-resistant stable materials for use in process vessels and crucibles for containment of (1) molten salts containing actinides and fission products, (2) molten actinide metals and chloride salts, and (3) molten non-actinide metals including zirconium.
- Analyze the effects of small additions of common anions ( $\text{Br}^-$ ,  $\text{F}^-$ ,  $\text{PO}_4^{3-}$ ,  $\text{I}^-$ ) to molten chloride salts for use in electrochemical recovery of specific transuranic elements.
- Develop the concept of a dry process for the treatment of spent TRISO fuel elements discharged from a high-temperature gas-cooled reactor.

### Engineered Product Storage

- Measure the thermal properties of the americium/curium storage form.
- Develop durable waste forms, fabricated at low cost, for the geologic disposal of krypton, iodine and tritium.
- Develop a concept of a storage form for the UREX+1 combined transuranic/lanthanide product stream and perform an evaluation of possible inexpensive container designs for temporary repository storage of this form.
- Assess the feasibility of incorporating the fission products barium, yttrium and rubidium in the steam reforming process for the production of the cesium/strontium storage form; measure the thermal properties of a prototype waste form comprised of non-radioactive constituents.

### Spent Fuel Treatment Facility Design/Process Technology Development

- Develop a comprehensive plant operations simulation code, perhaps using the ASPEN<sup>®</sup> framework, for evaluation of process technology options prior to the pre-conceptual design of the large spent fuel treatment facility. The code must provide for plant design parameter variation studies and produce a complete mass balance evaluation of all process streams for the chosen flowsheet and process technology. The code must also include provisions for the evaluation of process control, monitoring, and materials accountancy needs. Advanced graphical representations of processes and process equipment must be provided for maximum user benefit.
- Develop and demonstrate advanced on-line, near real-time analytical instrumentation for use in rapid and precise analysis of process streams, with the intention of providing a state-of-the-art system for the monitoring and control of process operations and the accounting of actinide materials for safeguards purposes.

## **1.2. Advanced Nuclear Fuel Development**

The listing of some R&D needs below is organized according to programmatic activity categories.

### Fuel design and analyses for advanced reactor concepts

- Define and analyze the fuel forms needed for novel concepts such as fast gas-cooled reactors (with high temperature capability), fast lead-alloy-cooled reactors (with high-density corrosive coolant), small-modular reactors (requiring long core life), and transmuters (with high TRU content, high helium generation, high burnup objectives). Different fuel geometries, such as plate-type fuels, dispersion fuels, and annular pellets are examples of new fuel design concepts of interest. Considerations such as strategically located burnable poisons and special getter materials in or around the fuel should be included. A proposal along these lines should include thermal and structural analyses for both normal operating conditions and accident conditions.
- Determine effective ways to getter cesium, silver, iodine, and tellurium in the high temperature conditions of advanced gas-cooled reactors. The purpose of this task is to

determine if cesium, silver, iodine, and tellurium can be gettered or otherwise removed at high temperatures, ~900-1000°C, in the core or hot duct of a gas cooled reactor. Small amounts of these elements are released during normal operation from failed fuel particles and from diffusion through the particle coatings. The major need is to prevent these materials from migrating to the power conversion unit of the reactor system and contaminating turbine and heat exchanger components, thus complicating maintenance. A secondary interest is to show that these elements can be tied up in the core to a high degree at higher temperatures (1400-1600°C) so that they are not available for release under accident conditions. The elements cesium and silver are of primary interest for this task, since they are the dose drivers for maintenance, but the control of iodine is also important since it is an off-site dose driver. This task might be part of the fuel safety envelope assessment discussed below.

#### Fuel safety envelope assessments

- Assess the safety envelopes of advanced fuel systems by analytical means. This should include identifying the key phenomenology for establishing the safety envelope, designing specific transient tests to address the important phenomenology, and performing some of the out of pile tests.

#### Assessment of surrogate materials

- Determine appropriate surrogate materials for addressing different fuels phenomenology as an early way to avoid using expensive and time-consuming real materials. This should include process development using surrogate materials and correlation of the surrogate-based processes with a limited number of actual material based processes (to be supplied by the National Laboratories). This project should include the definition and quantification of how surrogate materials could be effectively employed to accelerate in-pile or out-of-pile testing of specific phenomenology.

#### Fabrication process development

- Devise a low-temperature or low-heat fuel fabrication processes, specifically for Am-bearing fuels. Because of the high vapor pressure of Americium at typical sintering temperatures and during typical sintering times, a considerable fraction of the Am may be lost out of the fuel pellet. Either low temperature or high-temperature short duration sintering processes that meet the density and microstructure requirements must be developed. Laboratory testing of innovative processes can be carried out using thermodynamic surrogates (e.g. dysprosium).
- Devise remote fabrication and quality assurance processes for fuels containing high quantities of TRU. Fuels containing high-quantities of transuranics require remote fabrication and characterization. Innovative design concepts that minimize the cost of fabrication, minimize the waste/scrap generation and that meet the quality assurance requirements with high reliability are of considerable interest.
- Devise fuel fabrication processes and benchmark the modeling processes against known data. Process models that minimize the testing and that can be used for optimization are important for the program. The research may also include a semi-empirical set of correlations between the fabrication process parameters and fuel irradiation performance results.

The following three R&D areas are specifically related to TRISO fuel and coated particles used in dispersion fuels applications:

- Develop improved compacting techniques to fabricate coated particles. Compacts for the advanced gas reactor (AGR) program are currently being produced using the overcoating methodology developed by the Germans for the Julich graphite moderated reactor. The overcoat is the so-called A3 matrix of natural graphite (64 wt. %), synthetic graphite (16%), and thermosetting resin binder (20%). There are several key areas of study concerning fuel compacts that would lead to possibly higher quality compacts and a better understanding of the components used in making compacts. Currently only solvated phenolic resin thermosetting binders are used, but phenolics have potential negative health effects, so having a substitute material that has equivalent properties would be beneficial. Potentially, a new monomer could be used as a replacement for the currently used phenolic resin. Helium is used as a coolant in the AGRs, but it is unknown whether helium will adsorb on graphite, so it would be useful to know if any coolant will be lost in the graphite. Also, gases like xenon are evolved which may adsorb as well. Lastly, microstructural examination of the natural and synthetic graphites themselves by small angle neutron scattering would be beneficial because it would provide information on the surface chemistry of the graphites, and potentially their wettability or adsorptive capabilities.
- Determine the detailed reaction kinetics for chemical vapor deposition (CVD) processes and incorporation into MFIx. The hydrodynamics of a fluidized bed reactor used for coating uranium fuel pellets is being modeled using a widely accepted multiphase flow software package called MFIx (<http://www.mfix.org>). The code allows for inclusion of detailed chemical reactions but such information is not readily available for the CVD process. Reaction kinetics for the chemical vapor deposition of carbon and silicon carbide on uranium fuel pellets is a very complicated process, which can be broadly split into two categories: (1) Gas-phase reaction kinetics, and (2) Particle/Reactor walls surface reactions. The first part entails arriving at detailed chemical reaction steps for the formation of CVD precursors in the gas as a function of local gas-phase properties. The second part involves formulating the reaction steps governing the vapor deposition on the surface as a function of local gas and solid-phase properties.
- Conduct experimental and numerical investigations of 6-inch coater hydrodynamics. The objective of this activity is to explore the bed and distributor hydrodynamics of the 6-inch coater. This study should address the issue of scale-up to a process-size coater from similar program activities with 1- and 2-inch coaters. With development of a validated numerical model, parametric design simulations will be practical. One component of this project should be the fabrication of an experimental mockup section. This bed should be of a transparent material and be instrumented with an appropriate combination of video (low and high speed), pressure, acoustic, temperature and/or other sensors based on experience with the 1- and 2-inch coaters at ORNL. Experimental objectives include parametric studies of global hydrodynamics and particle mixing patterns, along with corresponding MFIx simulations.

#### Pre- and post-irradiation automated characterization methods

- Develop advanced characterization techniques that can be automated and that rely on non-destructive techniques (e.g. X-ray techniques). Fuel characterization before and



after irradiation is an important step to establish a qualified fuel for various reactor technologies. Characterization is an expensive process, especially when it is part of the post-irradiation examination.

### Design and instrument development

The following three suggested R&D areas augment the value from irradiation tests in reactors (e.g. ATR). The interest is in developing compact, remotely operated instruments that are tolerant to the radiation environment (e.g. neutron fluence and temperature).

- Develop and evaluate thermocouples for high temperature nuclear environments. The two most commonly used thermocouple types for nuclear applications at high temperature are Type “K” and Type “N”. Both have a high probability of failure when subjected to the fuel irradiation conditions for an extended period of time. The research should target identification of candidate materials, fabrication of the thermocouples, and testing.
- Optimize the gamma-ray detectors for the Advanced Test Reactor (ATR) fission product monitoring system. Fission product monitoring systems to confirm fuel performance and integrity are an essential feature of the Advanced Test Reactor (ATR) systems, specifically for Advanced Gas Reactor (AGR) fuel testing and qualification, and more generally for other advanced fuel testing and qualification. Since the AGR test plans call for multiple simultaneous test capsules, as many as 36 independent monitor systems may be required. These systems typically employ cryogenically-cooled High Purity Germanium (HPGe) detectors viewing a test gas effluent line. In early tests, failures of a single TRISO fuel micro-sphere must be reliably detected, while later experiments may require monitoring of fairly large particle failure fractions (perhaps 10%). The fuel irradiation tests will typically be two years in duration, so excellent system reliability is required.
- Develop methods to evaluate and limit fission product plating in ATR fission product monitoring system tubing. In fission product monitoring systems (see previous item) deployed earlier, a significant build up of reactive fission products on the walls of the fission product transport tubing and the fission product monitor spool piece was noted. This deposition of reactive fission products decreased the detection sensitivity of fission product monitors, complicated the accurate determination of fission product releases, and complicated system maintenance. Innovative research that leads to sample transport systems and/or monitor system sample spool pieces that allow little or no deposition of reactive fission products would be of great value to the AGR Fuel program, and proposals are encouraged. Also of interest are real-time signal processing techniques that overcome the effects of such deposition.

### Advanced mechanistic models and simulation tools

- Develop atomistic-scale to continuum scale models to replace the empirical modules in existing performance codes (e.g. FRAPCON for oxide fuels, PARFUME for TRISO fuels). Fuel development and qualification is an expensive process if one relies solely on testing and empirical knowledge. An important objective of the AFCI and GEN IV program is to enhance the capabilities of the fuel performance codes by replacing some of the empirical models with more mechanistic models based on first principles. The development of such models and benchmarking against available separate effect and

integral effect data would be valuable. Models applicable to ceramic, metal and composite fuels are all within the scope of the ongoing research.

- Develop a thermo-chemical model of a multicomponent TRISO fuel kernel that allows the analyst to determine the oxidation state of the fuel, additives, and fission products within the kernel as a function of burnup. This project should provide an estimation of the mobility of these materials and whether they pose a threat to particle integrity. The purpose of this task is to examine how kernels containing two or more chemical species or kernels coated with a thin layer of getter material may be used to control LEU coated particle fuel internal gas pressure and retain fission products. Previous work has examined a two phase kernel composed of  $\text{UO}_2$  and  $\text{UC}_2$ , which both controls particle CO pressure and oxidizes rare earth elements to reduce their mobility. Other kernel constituents such as ZrC may perform a similar gettering function and still others may be used to tie up specific fission products. Beyond control of oxygen potential, additives that limit the mobility of noble metals such as Pd would be of interest as these fission products attack the SiC layer.

#### Advanced cladding and matrix material development and characterization

- Develop advanced cladding material that can resist high fluences, high temperatures, and potentially corrosive liquids (e.g. Lead alloys). Advanced cladding concepts include non-metallic cladding, corrosion resistant cladding for lead alloy applications, high-temperature resistant cladding for fast-gas reactor applications and high-fluence and high-energy flux resistant cladding materials for fast spectrum applications. For transmutation fuels, the transmutation efficiency is directly tied to the achievable burnup without recycling. Typically, the fuel burnup is limited by the structural integrity of the cladding.
- Develop matrix materials that are radiation tolerant and that can resist high-temperatures (up to  $\sim 1000^\circ\text{C}$ ). The matrix materials must be compatible with the fuel particles and the coolant (in case of a cladding breach). A determination of the basic properties of such matrix materials is of benefit to all advanced reactor applications in the AFCI and GEN IV programs.
- Define and develop an appropriate ceramic matrix suitable for Inert Matrix fuels that is compatible with water and also amenable to aqueous reprocessing. The commonly used zirconia matrix for transmutation in LWRs is very difficult to recycle. The AFCI program is interested in matrix material candidates that can be recycled (e.g. MgO) but that are also compatible with the coolant under cladding breach accidents (e.g. hot water is very corrosive for MgO).
- Characterize graphite properties of advanced gas-cooled reactors after adsorption of fission products. The natural graphite contains impurities in the form of metallic inorganics that may act as active sites for adsorption of gaseous fission products like CO,  $\text{CO}_2$ , or other species. It is unknown whether the adsorption of such gases would incur structural damage to the matrix, so a study focused on the property changes of graphite after adsorption of fission products would be beneficial in predicting the quality of a fuel compact, as well as its lifetime in a reactor.

### 1.3 Transmutation Science and Engineering Technologies

The listing of some R&D needs below is organized according to programmatic activity categories.

#### Transmutation Physics

Analyze Doppler feedback sensitivity in the Los Alamos Critical Experimental Facilities (LACEF). In working with the laboratory scientists and engineers, develop an experiment using one of the critical assemblies at LACEF. Determine the potential for measuring small changes in reactivity with and without heated actinide samples in order to measure their temperature coefficient. Evaluate the magnitude of reactivity changes due to the presence of small quantities (~1 g) of minor actinide isotopes inserted into candidate critical assemblies at LACEF. Do this as a function of temperature of the minor actinide.

Develop a next-event estimator capability in MCNPX for neutral particles above the tabular region. Currently, the next-event estimator, which is a powerful variance reduction capability in MCNPX, works only in the energy region where tabular data exist. A very nice doctoral dissertation topic can be derived from developing the methodology needed to extend this capability to the energy region where physics models are used to derive reaction cross sections. Materials and Coolants for Accelerator Driven Systems (ADS)

Evaluate austenitic (316L/D9) and ferritic/martensitic (HT-9) steels with additional silicon content. Optimize for enhancing lead-bismuth eutectic (LBE) corrosion resistance and lessening radiation damages (embrittlement).

- Investigate surface implantation/treatment with plasma, electron beam and other advanced techniques for critical components to improve compatibility and performance.
- Investigate HT-9 secondary treatment, following the Russian IPPE procedures for EP-823 (spallation target window, fuel cladding and core structures in LBE systems), to make changes in thermal mechanical properties, microstructures, surface conditions, and LBE corrosion resistance .
- Using the DELTA loop, provide small corrosion samples for testing under controlled LBE temperature, flow and oxygen content conditions. Conduct post-test examinations of corrosion tested steel samples (metallography, X-ray, SEM, TEM etc for microstructure and composition analysis).
- Apply electric impedance spectroscopy (EIS) to in-situ monitoring of LBE corrosion and protective oxide film formation.
- Conduct advanced materials screening (refractory metals and alloys, ceramics and composites) for high performance systems (e.g. determine availability, fabrication processes, joint techniques, and thermal-mechanical properties in a non-radiation environment).

- Determine structural properties of potential structural and fuels materials as a function of radiation damage, helium production, and hydrogen production at temperatures of interest for Accelerator Driven Systems (ADS) applications.
- Develop atomic-scale radiation damage models for extrapolating structural properties of potential structural and fuels materials.
- Develop and test new radiation damage resistant alloy formulations.
- Measure the fatigue or fatigue crack growth resistance of ferritic/martensitic alloys at prototypic temperatures of 400-600 C.
- Determine the applicability of nanostructured materials to radiation resistant applications. Determine the microstructural stability at prototypic temperatures of 400-600C.
- Determine the effect of single crystal orientation on radiation damage in BCC iron.
- Determine the effect of grain boundary orientation (coincident-site lattice (CSL) enhanced) on LBE corrosion.

#### LBE Research

- Model the corrosion kinetics in multi-branch and multi-section reactor-like LBE systems, including the coupling of chemical reactions, species transport and coolant flow. Use oxygen as the controlling agent.
- Develop sensors for mapping temperatures, conducting non-destructive tests for structural integrity, and recording ultrasonic Doppler velocimetry in a radiation environment.
- Investigate oxygen partial pressure control via moist hydrogen gas mixtures for coolant conditioning.
- Conduct an experimental study of oxidation mechanisms and kinetics and their dependence on surface/structural conditions.
- Examine the effect of proton irradiation on protective oxide layer and film formations in LBE systems to evaluate the impact of a proton beam on the corrosion rates in LBE systems.
- Design and commission a lead-bismuth loop facility for UNLV. Maximize the use of the facility by designing a hydraulic benchmark and test campaign, designing a thermal-hydraulic benchmark and test campaign, and designing a materials performance campaign for the LBE loop at UNLV.

- Analyze available thermal-hydraulic experimental results from LBE research programs (e.g. from DELTA at LANL, KALLA at FZK, etc), and evaluate from these data the dependence of heat transfer and thermal hydraulics on coolant chemistry.
- Develop an ideal manufacturing process for producing high quality corrosion probes. Then produce such test probes and test them in an operating environment to examine their performance in a LBE environment (typical temperature and radiation environmental conditions).
- Develop an ideal manufacturing process for producing high quality oxygen probes. Then produce such test probes and test them in an operating environment to examine their performance in a LBE environment (typical temperature and radiation environmental conditions).
- Adapt and/or build computer simulation codes/systems for transient and safety analysis of LBE systems, benchmarking results with data from experimental facilities.
- Develop LBE system decontamination and decommissioning (D&D) requirements.

#### **1.4 Advanced Fuel Cycle Systems Analysis**

- Design and analyze advanced fuel cycles for LWRs, including BWRs.
- Develop an advanced assembly for TRU recycle in LWRs, including a safety assessment.
- Determine the effect of nuclear data uncertainties on fuel cycle evaluations. Determine the feedback for nuclear data needs.
- Develop core designs for low conversion ratios, or core designs that allow for variable conversion ratios.
- Identify and assess the repository benefits of advanced fuel cycles.
- Determine the effect of uncertainties on repository benefit assessments.
- Conduct dynamic fuel cycle scenario studies to develop an understanding of the issues in the transition from thermal reactors to a mixed thermal/fast reactor fleet, or a fleet in which the majority of reactors are fast and/or accelerator-driven.
- Articulate and assess the impacts of socio-economic factors in fuel cycle deployment.
- Optimize the use of key resources, e.g., repository capacity and uranium ore, in the long term for advanced fuel cycles.
- Evaluate the optimal use of fast reactors and accelerator driven systems.

## 2. Generation IV Nuclear Energy Systems Initiative

### 2.1 Supercritical Water-Cooled Reactor

The listing of some R&D needs below is organized according to the six categories outlined in the summary:

#### Baseline Design for the SCWR Core and Reactor Coolant System

- Develop a credible thermal, neutronic and mechanical design for the fuel assembly and vessel internals, as well as a reactivity control system based on control rods and burnable poisons. The objective is to establish a baseline conceptual design for the core and reactor coolant system to which all other activities (e.g., materials, safety, etc.) can relate. It is well known that SCWRs require a dedicated moderator to realize a thermal-spectrum core because of their relatively low coolant density. Several approaches are being investigated in Japan, Europe, the U.S., Canada and Korea, including the use of water rods or low-temperature heavy water in a separate moderator tank. The mechanical design of the fuel assembly with water rods (the current U.S. reference design) is fairly complicated. On the other hand, the use of heavy water requires the development of a very high-temperature high-pressure tube design. Therefore, it is desirable to explore innovative designs that could overcome such shortcomings. For example, the use of TRIGA-type hydride fuels would eliminate the need for a separate moderator, while the use of a solid moderator could simplify the reactor internals.
- Conduct neutronic/thermal-hydraulic coupled analyses for the fuel assemblies, recognizing that the density distribution of the supercritical water coolant affects the neutron flux distribution. The operating temperatures, linear heat generation rates, core geometry and flow rates need to be identified. Compare results to the current U.S. reference design to evaluate relative merits.
- Conduct depletion calculations to show that acceptable discharge burnups can be achieved for reasonable beginning-of-life enrichments. Compare results to the current U.S. reference design to evaluate relative merits.

#### Basic Thermal Data for the SCWR

- Conduct experiments to accurately establish the heat transfer coefficient to supercritical water coolant under a variety of heat transfer regimes—including upflow, downflow and horizontal forced convection at high and low mass fluxes, buoyancy assisted forced convection, pure free convection, and deteriorated heat transfer. Transition from one regime to another including the depressurization to two-phase flow conditions of an initially supercritical fluid should be correlated in terms of dimensionless groups facilitating the comparison among different fluids, geometries and flow conditions. Also, in bundle geometry where a circumferential symmetry does not exist, provisions should be made to measure the azimuthal variation of the heat transfer coefficient. Special effects such as flow channel shape, grid spacers, and non-uniform heat flux should be quantified. Both actual SCW and supercritical surrogate fluids (e.g. CO<sub>2</sub> and Freon) can be explored in this task.

Surrogate fluids are convenient to minimize cost and time in constructing and operating the experimental facilities. On the other hand, SCW provides a direct representation of the SCWR behavior without the need for scaling of the thermo-physical properties. While considerable information exists on heat transfer to supercritical water in round tubes for fossil boilers, little is known about the effect of the geometry and fluid conditions typical of the SCWR core. Therefore, this task addresses the critical issue of measuring heat transfer to supercritical water at prototypical SCWR conditions and to develop the tools to predict the SCWR thermal behavior. The new data made available should be incorporated into existing computational codes such as RELAP, FLUENT, etc., for use in the SCWR analysis.

- Construct and operate an experimental facility to obtain crucial data for critical (or choked) flow at supercritical conditions. Critical (or choked) flow phenomena are of great importance in designing/operating the reactor safety/relief valves and the automatic depressurization system, as well as in the analysis of LOCA events. The envisioned experimental facility would consist basically of a pressure tank and a discharge nozzle. The stagnation conditions in the tank as well as the diameter and length of the discharge nozzle should be systematically varied. Blowdown experiments should be performed in this facility. Direct experimental measurements of the temperature and pressure along the discharge nozzles, and of the void fraction and flow rate at the nozzle outlet should be obtained. These data will enable accurate benchmarking of existing critical-flow models and should be incorporated into existing computational codes such as RELAP, FLUENT, etc., for use in the SCWR analysis.

#### SCWR Safety Systems and Containment Design

- Conduct a conceptual design and analysis of the SCWR containment and safety system, recognizing that the thermal inertia of the primary system is significantly lower than for an LWR. This should include the reactor protection system, the residual heat removal system, the over-pressurization protection system, the ECCS, reactor shutdown system, steam and pressure relief systems. A general safety strategy to cope with postulated sequences (e.g., depressurization vs. high-pressure emergency coolant injection) should be defined for accidents such as LOCAs or LOFAs. It will be necessary to determine if this strategy can be implemented with active or passive safety systems. This task should focus mostly on assessing the applicability to the SCWR of passive safety systems developed for advanced LWRs (e.g., ESBWR, AP-600) including isolation condensers, gravity-driven cooling systems and a passive containment cooling system.

#### SCWR Stability Analysis

- Develop analytical models to predict the onset of instabilities of the density-wave, coupled thermal-hydraulic/neutronic and natural-circulation type. The models should capture the effect of important variables such as axial and radial power profile, moderator density and fuel temperature reactivity feedback, fuel rod thermal characteristics, coolant channel hydraulic characteristics, heat transfer phenomena, and core boundary conditions (including the effect of direct or indirect cycles). Mitigating effects like orificing, insertion of control rods, and fuel modifications to obtain appropriate thermal and/or neutronic response time constants should also be assessed using analytical simulations. Parallel channel instabilities should be investigated as well as instabilities during start-up and partial load operation. Also, experimental data derived from existing supercritical water and/or CO<sub>2</sub> loops should be incorporated into the new analytical models. Since SCWRs present the possibility of various types of instabilities, namely, density-wave instabilities, coupled

thermal-hydraulic/neutronic instabilities, and natural circulation instabilities, it is necessary for any given design to show that either the oscillations do not occur during normal operation or that if they do, they can be detected and suppressed in a safe manner. Finally, oscillations under accident conditions must also be considered, e.g., under anticipated transient without scram conditions. The overall objective of this task is to achieve a better understanding of instability phenomena in SCWRs, the identification of the important variables affecting these phenomena, and ultimately the generation of maps identifying the stable operating conditions of the different SCWRs designs.

### SCWR Control and Start-up

- Develop a strategy for controlling the main reactor variables, e.g., core power, coolant pressure and temperature. A possible control approach might be controlling the core power by the control rods, the pressure by the turbine throttle valve, and the coolant core outlet temperature by the pump flow. However, other approaches are possible and could be better. Equally important is the issue of plant start-up from cold conditions. In fossil-fueled supercritical plants, two different start-up approaches are possible--including one with constant pressure and one with sliding pressure. Implementation of these approaches in a SCWR plant will likely require installation of dedicated out-of-vessel components (e.g., a flash tank for constant-pressure start-up, a steam separator for sliding-pressure start-up). Therefore, besides the technical feasibility of these start-up approaches, this task should assess the cost impact of one versus the other, as well as the sizing of these components.

### Materials and Chemistry in the SCWR

- Establish a systematic basis for evaluating corrosion and stress-corrosion cracking patterns of candidate fuel cladding and structural materials for SCWR application. Unirradiated, proton-irradiated and neutron-irradiated alloy coupons should be exposed to supercritical water at controlled temperature, pressure, oxygen concentration, electric conductivity and pH to assess their susceptibility to corrosion and stress-corrosion cracking. These data will form a rational basis for down-selection to a limited set of promising alloys, which will be more aggressively tested/developed later in the program. In addition, an accurate understanding of water radiolysis at SCWR conditions should be pursued by means of in-pile loops and out-of-pile pulse radiolysis facilities. This task is important because the generation of oxygen, hydrogen peroxide, and hydrogen gas by radiolysis and the high solubility of these gases in supercritical water could result in higher corrosion and stress corrosion rates than experienced with other reactor designs. In addition, radiation may accelerate or assist corrosion and/or stress corrosion cracking in the reactor region. Despite the successful operation of numerous supercritical fossil power plants worldwide, the existing data base on corrosion and stress corrosion cracking of austenitic stainless steels, nickel-based alloys and ferritic-martensitic steels in supercritical water is very sparse and is non-existent for irradiated alloys.

## **2.2 Next Generation Nuclear Plant**

The listing of some R&D needs below is organized according to programmatic activity categories.



## 2.2.1 Reactor Neutronics and Thermal-Hydraulic Analyses for the NGNP

### Advanced Neutronic Core Design Analysis Tools

- Evaluate the capabilities and make improvements to the multi-group cross section generation, neutron transport, depletion, kinetic, and fuel management optimization analysis tools currently available to support the NGNP design. This effort should also include an assessment of the various code capabilities for accuracy, traceability, verification, documentation, and the software quality control. It will be necessary to build new models, run verification problems, create numerical benchmark problems for code cross comparisons, identify benchmark criticality problems, and run benchmark test problems to compare the models with experimental data (k-effective, decay heat, radionuclide isotopes, etc). Some of the national/international benchmark problems and databases that may be used include Fort Saint Vrain, Peach Bottom, THTR and AVR, HTTR and HTR-10, AGR/MAGNOX reactors, PROTEUS, DRAGON, and Graphite Criticality benchmarks from the International Criticality Safety Benchmark Project.

### Testing & Validation of the NGNP Thermal-Hydraulic Analytical Methods

- Evaluate the accuracy of thermal-hydraulic codes in modeling the behavior expected in the NGNP. Specifically, RELAP5-3D and FLUENT codes should be benchmarked against existing data relating to the design and operation of high-temperature, gas-cooled reactors. Over the past four years, RELAP5-3D has been enhanced to provide the basis for modeling several different Generation IV designs, including the Supercritical Water Reactor, Lead-Bismuth Cooled Reactor, Gas Cooled Fast Reactor, as well as the Very High Temperature Reactor. It has also been coupled to the FLUENT CFD code to enable a domain decomposition approach to modeling complex gas reactor coolant systems. Experimental data from a number of test facilities is available to benchmark these codes. Among these are the HTTR RCCS Mockup Facility experiments (Japan), SANA-1 facility experiments (Germany), Bugey-1 Arret Program (France), HTTR safety tests (Japan) and HTR-10 tests (China). RELAP5-3D and FLUENT should be used to model these facilities and comparisons to experimental data should be made and analyzed to provide guidance on future code refinements and uncertainty analysis.
- Develop and/or modify the turbulence models in FLUENT so that they properly model the new situations and conditions of the NGNP. One of the most difficult hurdles to the proper use of CFD codes is the turbulence modeling. Therefore, these codes often provide the user the choice of a number of different models, but it is also often unclear as to which models are appropriate for which simulations. There is an urgent need to find the best models or develop new turbulence models to fit the conditions of NGNP.

### Experiments Supporting Thermal-Hydraulic Code Assessment and Development

- Conduct separate effects experiments using prototypic or scaled geometries, addressing both normal operating and accident conditions, possibly using more than one coolant. The objective of the experiments should be to generate heat transfer and fluid flow data that can be used to assess the system codes. Depending on the results of the assessments, new correlations and models may need to be developed for implementation in the system codes.

Experiments may also address the integral behavior of portions of the plant, such as passive heat removal from the core to the ultimate heat sink. Appropriate equations of state for the coolants may also need to be developed for implementation in the analysis codes.

#### Models and Tests for Air-Cooled Passive Decay Heat Cooling Systems.

- Develop models and conduct confirmatory tests to understand the performance of alternative passive air-cooled decay heat cooling systems at vessel temperatures as high as 800 degrees C. The NGNP concepts propose to use passive air-cooled decay-heat cooling systems. While these systems have been extensively investigated for gas-cooled and sodium-cooled reactors at lower temperatures, they have not been investigated at higher temperatures. NGNP systems may have much higher operational, accident, and beyond-design-basis-accident vessel temperatures.

#### Development of Better Air Ingress Analyses Tools

- Develop a credible air ingress analysis capability that would include a more powerful tool, such as FLUENT 6.1, to model the corrosion of graphite under real reactor conditions. This could be linked to RELAP or GRSAC. Unfortunately no benchmarks presently exist; therefore, cooperation with Germany in their upcoming tests would be desirable. This should be applicable to both prismatic and pebble bed reactors. Experiments to validate selected thermo-chemical models to describe the effects of air-ingress into a pebble bed or prismatic NGNP would be desirable.

#### Methods Development for Modeling the NGNP Balance of Plant

- Develop and validate the capability to represent gas cooled reactor balance-of-plant components not represented in the current systems codes, like compressors and recuperators. Most of the computer codes being used today for analyzing the performance of nuclear reactor systems were developed for light water reactors. While the component models in the current codes can be used to approximate the behavior of gas reactor components for scoping analyses, more appropriate models are needed for detailed safety analyses.

#### Fuel Particle Flow Velocity and Distribution for Fuel Management in the High Temperature Pebble Bed Reactor

- Conduct an experimental and modeling study to determine the feasibility of various nuclear fuel management designs for the pebble bed version of the NGNP. The fuel management scheme for the gas-cooled pebble bed NGNP requires that the fuel will be recycled approximately 10 to 15 times to achieve the economics of operation needed and provide the necessary burnup. A workable fuel management program requires that the reactor vessel must have a predictable flow of pebbles through the system. However, studies have shown that all hopper and process equipment handling granular and powder materials inherently have a velocity distribution across them as they flow in a converging hopper section of a bin. These velocity profiles have been observed to be faster in the center of a hopper than at the edge of the hopper. In addition to this normal variation, the ceramic pebbles will tend to get hotter as their surface temperature increases as they travel downward in the reactor vessel with the concurrent coolant flow and this may affect their flow behavior. Also, coolant pressure gradients and uneven surcharge pressures caused by conical piles of material

feeding the reactor may cause local changes in velocities of the pebbles. This situation can make the fuel management modeling of the reactor especially challenging if this behavior is not understood. Considerable experimental work has been done in South Africa on this problem and the data from that work may be available for incorporation into the models.

#### Decay Heat Cooling for the Molten-Salt Cooled NGNP

- Evaluate the performance of alternative higher-temperature air-cooled passive decay-heat cooling systems and conduct experimental validation of such systems. The Advanced High Temperature Reactor, the alternative molten-salt-cooled NGNP, may reach vessel temperatures as high as 800 degrees C. While air-cooled decay heat systems have been developed for gas-cooled and sodium-cooled reactors, the existing data is for lower temperature systems. An understanding of these systems at higher temperatures is required.

#### Improved NGNP Severe Accident Analysis Modeling

There are a number of severe accident modeling tools that can be used for analyzing the NGNP, including GRSAC, MELCOR, and SCDAP/RELAP, but all need improvement to be confidently used.

- Evaluate the applicability of MELCOR for confident use in analyzing severe accidents in the NGNP. MELCOR is an integrated fast-running code developed by the U.S. NRC for the analysis of severe accidents in light water reactors. Originally a probabilistic risk assessment code, MELCOR has undergone extensive development and is now capable of modeling the thermal-hydraulic response in the reactor coolant system, containment and confinement buildings, the behavior of the core, fission product transport, and other phenomena necessary to evaluate the severe accident progression out to the source term. In recent efforts, the code has shown the potential for advanced reactor and nonreactor applications.
- Evaluate the applicability of GRSAC for confident use in analyzing severe accidents in the NGNP. GRSAC is an integrated fast-running code developed by ORNL for analysis of severe accidents in gas-cooled reactors. GRSAC has undergone extensive development over the years and is capable of performing detailed analysis of the severe accident progression in gas-cooled reactors. However, many of its capabilities are empirical and its models are not always sufficient for all the problems of interest. Hence, a key part of this task would be to remove reliance on empiricism to the extent possible.
- Evaluate the applicability of SCDAP/RELAP5 for confident use in analyzing severe accidents in the NGNP. This tool was developed and used by the NRC and DOE for the analysis of severe accidents in current generation and advanced light water reactors. The code utilizes the sophisticated thermal-hydraulic modeling capabilities of the RELAP5 code coupled with the detailed mechanistic modeling of core degradation phenomena to predict the complex behavior occurring during a severe accident in a nuclear reactor. Because of its unique capabilities, the SCDAP/RELAP5 modeling capabilities have been extended in several areas to allow modeling of severe accidents in various advanced reactor designs, including high-temperature gas-cooled reactors, supercritical-water reactors and liquid-metal cooled reactors. Some of the capabilities added include (1) oxidation of graphite structures in the presence of air and/or water vapor, (2) forced convection heat transfer and flow losses through pebble-bed reactor cores, (3) thermal and mechanical properties for various

advanced reactor fuel/cladding materials, (4) improvements in the RELAP5 computation of supercritical water properties and heat transfer correlations, and (5) modeling of molecular diffusion of air into the reactor system from a primary system pipe break (in progress). These improvements, along with continued improvements in the RELAP5-3D code to which the SCDAP severe accident model is linked, provides a powerful tool for analysis of severe accidents in various advanced reactor designs. However, the current question is its applicability to the NGNP design.

## **2.2.2 Materials Related to the NGNP Project**

### Graphite Irradiation Induced Swelling and Shrinkage

- Evaluate the irradiation induced swelling and shrinkage of the core graphite reflector and supports. The graphite previously used in the Fort St. Vrain and other high temperature reactors (H-451) is not available and new graphites need to be qualified. Fortunately, likely potential candidates currently exist, including fine grained isotropic, molded or isostatically pressed, high-strength graphite suitable for core support structures, fuel elements, replaceable reactor components, and large permanent reflector components (Carbone USA grade 2020 and Toyo Tanso grade IG-110). Some irradiations of relatively small samples of the new graphites are underway at ORNL, but additional irradiations may also be needed. Also, highly irradiated graphite reflector blocks from Fort St. Vrain are available for examination and some useful information may be obtained from that material.

### Control Rod Cladding and Guide Tubes Materials

- Test and evaluate candidate materials for the control rod cladding and guide tubes as well as the materials that support the insulation in the hot duct and upper plenum. These materials will be exposed to extremely high temperatures during certain accident situations. Composites of either carbon/carbon ( $C_f/C$ ) or silicon-carbide/silicon-carbide ( $SiC_f/SiC$ ) could be potentially used to fabricate these components. Work at PNNL and elsewhere has shown that composites of  $SiC_f/SiC$  have the potential for excellent radiation stability. The continuous fiber architecture, coupled with engineered interfaces between the fiber and matrix, provide excellent fracture properties and fracture toughness values on the order of  $25 \text{ MPa m}^{1/2}$ . The strength and fracture toughness are independent of temperature up to the limit of the fiber stability. Also, these fiber/matrix microstructures impart excellent thermal shock and thermal fatigue resistance to these materials so start-up and shutdown cycles and coolant loss scenarios should not induce significant structural damage. However, the effective transverse thermal conductivity is relatively low. The R&D to be performed would consist of additional irradiations and thermal and mechanical property tests of relatively large components.

### IHX Materials

- Evaluate candidate materials for the intermediate heat exchanger (IHx). The viability of the NGNP as a heat source for hydrogen generation will depend on the availability of heat exchangers that can operate in the 900 °C and above temperature range. For the 900 °C range, nickel base and/or cobalt-based super alloys (solid solution strengthened or ODS) are attractive based on their use in aircraft engine applications. For temperatures above 1000 °C there is no current metallic material that will be suitable, although refractory alloys

have been suggested. More likely, in this temperature range a ceramic-based component will be required. In the case of metallic materials, there are several candidate materials including Alloy 617, Hastelloy X and XR, and MA958 among others. However, these materials have not been used in compact heat exchanger applications and a significant development effort will be required to both qualify these materials from a materials performance point of view as well as from a processing point of view. A key element in the development and qualification of these, and similar materials, for compact heat exchanger design will be the ability to bond these materials in both thick and thin sections. R&D in the area of diffusion bonding of these materials would provide key information related to the potential use of these materials in compact heat exchanger applications.

*Tests Required To Quantify the High Temperature Materials Interactions and Potential Degradation Caused By Low Levels of Impurities Transported In the Helium Coolant*

- Conduct experiments to quantify the high temperature materials interactions and potential degradation caused by low levels of impurities transported in the helium coolant. The internals of the reactor and all the internals in the primary system will operate in a high temperature helium environment. It is known from prior studies that metallic materials that are exposed to low levels of  $H_2$ ,  $H_2O$ ,  $CH_4$ ,  $CO$  and  $CO_2$  contaminants in high temperature helium can be carburized or decarburized on the surfaces. These impurities result primarily from the hot graphite reacting with free  $O_2$  and much of the  $CO_2$  in the gas stream. These reactions, depending on rate and other factors, can substantially affect the long-term mechanical properties of the metallic components such as fracture toughness, fatigue, and creep rupture. Because of the low partial pressures of the impurities and the reaction characteristics of the exposed material at high temperature, the oxidation/carburization potentials are complex and are established by the individual impurity catalyzed reactions on the surface. Some data regarding high temperature materials stability under these conditions currently exist; however, most of the materials that will be required for fabrication of the NGNP primary system have not been thoroughly evaluated. The mechanical properties of these materials need to be evaluated following high temperature exposure to hot helium with appropriate impurity levels to establish baseline data where it does not currently exist.

*ASME Codification of Alloy 617, Mod 9Cr-1Mo Steel, and Hastelloy X*

- Determine the data and evaluations needed for ASME codification of Alloy 617, Mod 9Cr-1Mo steel, and Hastelloy X. These alloys will almost certainly be required for the fabrication of key NGNP structural components in the primary system. None of these alloys, however, are currently included in Subsection NH of the American Association of Mechanical Engineers (ASME) Boiler and Pressure Code. Subsection NH provides Section III (nuclear service) high-temperature design rules for the construction of Class 1 components that have metal temperatures that exceed those covered by Subsection NB and Tables 2A, 2B and 4 of Section II, Part D, Subpart 1 of the ASME Code. Much of the required data set for these materials for inclusion in the ASME Code has been previously obtained and for some of these materials the data have been assembled as draft ASME Code cases. However, in some cases, this effort was terminated several years ago due to the lack of available program funding and interest. The prior draft ASME Code cases need to be reviewed and updated on an urgent basis. In some cases, particularly for Alloy 617, additional mechanical property, weldment, stress rupture, and fatigue data, aging effects information, and further structural design methodology information is required. Because Class 1 components cannot generally be approved for nuclear service without inclusion in Section III of the ASME Code,

and these are important alloys that will be used for fabrication of components in the primary system of the reactor, it is important that this work be initiated.

### Improved Strength for High Temperature Metallic Components

- Develop a research plan on alloying, materials processing, or coating techniques to improve high temperature mechanical or environmental materials performance. The NGNP metallic components may reach operating temperatures as high as 1000 °C with transients to 1200 °C. Metallic components with ASME code cases are not qualified for these temperatures and many common high temperature materials are not expected to have adequate strength or environmental resistance at these temperatures. This R & D task should define the techniques to improve performance, along with the methods to evaluate the improvements in performance.

## **2.3 Lead Alloy Liquid-Metal-Cooled Fast Reactor**

The listing of some R&D needs below is organized according to programmatic activity categories.

### Studies of three-dimensional natural circulation in Pb and/or Pb-Bi

Measurements of flow and convection parameters and/or correlations are of interest to enable modeling of natural-convection heat transport in various core designs under various conditions. Measurements of parameters that affect gas-injection lift pumping are also important for designing such a system in an LFT and for considering the probability and impact of any bubbles getting into the core.

- Conduct theoretical and engineering systems studies to determine the stability of natural circulation for autonomous power small modular LFRs.
- Conduct experiments to determine the natural circulation heat-transfer and pressure drop correlations.
- Investigate the effects of gas injection (i.e., lift pump action) upon the enhancement of flow and heat transport.
- Conduct experiments and perform data analyses on natural circulation and its stability, gas injection, simulation of system transients, and power profile effects.

### LFR Materials Screening (in collaboration with materials specialists at the national labs)

There is a need for identification of additional materials or materials treatments for enhanced Pb/LBE compatibility and for understanding the Pb/LBE corrosion processes such that corrosion mitigation strategies can be identified.

- Identify new or modified materials for successful application in Pb and Pb-Bi-eutectic systems. This could include alloying additions (such as Si additions to U.S. stainless steels), surface modification, or new fabrication techniques. Material performance issues include Pb/LBE compatibility, high-temperature strength, and resistance to irradiation-induced degradation.

- Perform experiments to characterize candidate materials, including bulk and surface considerations, plus corrosion screening tests. Take advantage of collaboration on existing experimental capabilities, such as the LANL DELTA loop and/or the ANL Pb/LBE corrosion equipment.
- Determine strategies for eliminating or relaxing oxygen control requirements for the compatibility of steels with Pb/LBE.
- Determine the irradiation effects on LFR candidate materials, including the effects of Pb/LBE corrosion.

#### Core Physics and Thermal-Hydraulics Design (in collaboration with ANL and LLNL)

Opportunities exist to conduct parametric studies of certain parameters or to develop detailed models of key features that often cannot be effectively addressed in the focused efforts at the laboratories.

- Conduct core design studies, including neutronics and/or thermal-hydraulics analysis, for small modular LFRs--with emphasis on achieving long core life. An assessment of reactivity effects should be included.
- Establish a core structural design to provide thermostructural reactivity feedback as required for passive safety and semi-autonomous load following.

#### LFR Energy Conversion Technology Studies

This task should be directed toward determining the benefits of coupling various conversion technologies with an LFR system and toward determining the interface requirements of such coupling.

- Assess proposed technologies for conversion and utilization of heat from a small modular LFR. Emphasis should be on determining the potential for increased conversion efficiencies, determining requirements for such systems, and proposing R&D priorities.

### **2.4 Gas-Cooled Fast Reactor**

The listing of some R&D needs below is organized according to programmatic activity categories.

### GFR Systems Design and Safety

The system design of the GFR will be affected by the choice of primary coolant, whether a direct or indirect power conversion cycle is used, and the core geometry (i.e. block, plate, pebble, etc.).

- Identify and assess the alternative GFR design features that fulfill Generation IV goals and criteria.
- Conduct a safety analysis for the reference GFR system and its alternatives.
- Develop and validate computational tools needed for the design and the analysis of operating transients (design basis accidents and beyond), including benchmarking against experimental data. This should also include the specification of required test facilities to obtain missing experimental data for the qualification of calculation tools.
- Conduct thermal-hydraulic analyses of current safety system designs, i.e., model development and transient analysis using semi-passive decay heat removal systems (this does not exclude the development of new designs, given they meet the goals of the system).
- Conduct initial PRA studies to determine the best safety systems (or combination of systems) that satisfy Gen IV goals in safety and reliability.
- Conduct a neutronic/physics core design analysis, including an analysis of reactivity coefficients during accident conditions and reactivity limited burnup.

### GFR Fuels, In-Core materials, and Fuel cycle

The fuel and fuel matrix/cladding to be used becomes a key issue in the development of the GFR. The trade-off between high conductivity and high temperature capabilities has led to the choice of ceramics, including refractory ceramics. The reference fuel matrix for the Generation IV GFR is a cermet dispersion fuel, based on a balance between conductivity and high temperature capability. The reference fuel designs are based on dispersion fuels (either as fibers or particles) in an inert plate/block type matrix, with options to use particle fuel in an inert pebble matrix, or solid solution fuel clad in a refractory ceramic (e.g., SiC/SiC composites). The reference fuels chosen for the GFR are UN and UC because of their high heavy metal density, high conductivity, and minimal impact on neutron spectrum (although limited irradiation data exists). The matrix/cladding materials are dependent on the coolant and operating temperatures, and can be classified into three categories: ceramic (for high temperatures), refractory metal (for modest to high temperatures), and metal (for modest temperatures). As the fuels are of ceramic composition, the resulting fuel forms can be classified into two categories: cermet and cermet. The in-core materials will have to withstand fast-neutron induced damage and high temperatures; up to ~1600°C during abnormal situations. Ceramic materials are the reference, and composite cermet structures or inter-metallic compounds will be considered as a backup. Efforts are currently being focused on the most promising carbide ceramics (preferred option): SiC, ZrC, TiC, NbC; or other materials like nitrides (TiN, ZrN), oxides (MgO, Zr(Y)O<sub>2</sub>) and possibly Zr, V or Cr based metallics as part of the CER/MET composite inert material, or intermetallic compounds like Zr<sub>3</sub>Si<sub>2</sub>.

- Develop innovative matrix material fabrication techniques for ceramics of interest.



- Model the fuel performance using UC and UN in ceramic matrices (specifically thermo-chemical).
- Conduct iron irradiation/implantation of ceramics (particularly heavy ion irradiation).
- Conduct UC and UN oxidation studies (e.g. air ingress, CO<sub>2</sub> ingress).
- Measure missing thermo-mechanical/physical properties for those ceramics of interest (e.g. carbides and nitrides).
- Conduct joining/welding studies of candidate materials (both ceramic and metallic).
- Conduct supercritical CO<sub>2</sub> corrosion studies on materials of interest (both ceramic and metallic).
- Conduct supercritical CO<sub>2</sub> radiolysis studies (decomposition and recombination rates).
- Conduct a preliminary assessment of the GFR fuel cycle (including flow sheet development, physics/neutronics analysis of equilibrium cycle, and possible surrogate material experiments).

## **2.5 Design and Evaluation Methods Development**

The listing of some R&D needs below is organized according to programmatic activity categories.

### **Design and Safety Analysis Methods**

- Develop an experimental data base of high-fidelity, multi-dimensional experimental fluid dynamics and heat transfer data suitable for qualifying the capabilities of current generation computational fluid dynamics (CFD) software. These data are needed for each of the different coolant types and flow regimes that are employed in Generation IV systems. Data for natural convection systems, including their transient startup and shutdown, are of particular interest given their importance for verifying passive safety features of Gen IV systems.
- Develop a general purpose two-phase (multi-field and multi-component) CFD and heat transfer simulation capability, applicable to different Generation IV coolant types and with capacity to account for transport between phases. Such capability is needed to address multi-dimensional design challenges in the development of compact and highly efficient components for a number of Gen IV system concepts. Applications would include development of energy conversion system components as well as analyses supporting primary system design. The capability should probably be developed as an extension of the existing multidimensional CFD software from the research or commercial sectors and must be suitable for analysis of reasonably complex geometries such as those found in nuclear power plant components. Capabilities for simulation of transients for both forced and natural convection systems are essential.
- Develop lattice physics capability for generation of accurate homogenized, few-group parameters for use in physics analysis of graphite-moderated reactors using coated particle fuel types. The capability must provide adequate representation of the multiple

heterogeneous nature of such fuel and should be applicable to generation of homogenized parameters that reflect the operational state history of each homogenized region, as well as the relevant characteristics of neighboring regions.

- Develop capability for accurate neutronic and fuel depletion analysis of systems with mobile-fuel (e.g., the pebble bed variant of the VHTR). Develop reliable estimates of the nominal values and uncertainties of predicted depletion-dependent parameters such as the core multiplication factor, power distribution and reaction rate distributions. The capability should rigorously account for the stochastic nature of the fuel motion in the derivation of uncertainty estimates and associated confidence intervals.
- Demonstrate improvement in the accurate and efficient prediction of the neutronic behavior of Generation IV systems as a function of fuel depletion and accounting for in-core and ex-core fuel management operations. The improved methods should enable more accurate and efficient estimation of both global and detailed neutronic parameters and should be amenable to increased automation to facilitate their use in designing and operating Generation IV systems. Accurate prediction of neutronic characteristics relevant to materials damage (e.g., fast fluence, DPA, gas generation rates) for both in-core and ex-core structures is of particular interest. Targeted improvements include reducing errors associated with spatial homogenization and group condensation, representation of whole-core transport effects, and better representation of the reactor's operational history and current state.
- Identify and substantiate needs for new evaluations or measurements of nuclear data, through systematic assessments of biases and uncertainties in predicted physics characteristics of Generation IV systems. These assessments are expected to include identification of relevant benchmarks (ideally based on measurement), comparison of predicted and measured physics parameters, identification of the data significant to observed discrepancies, assessment of the uncertainties in these data, and demonstration of the incentive to reduce their error/uncertainty. Achievable improvements should be quantified for predicted reactor physics parameters, safety coefficients, and depletion-dependent nuclide inventories and radiation emission characteristics.
- Develop and qualify efficient methods for nuclear data sensitivity analysis for thermal spectrum Generation IV systems (VHTR and SCWR). Methods should account for effects of data homogenization and minimize the need for explicit recalculation of the effects for each data perturbation.
- Improve Monte Carlo capabilities for whole-core and shielding applications, e.g. through increasing the reliability of variance estimates, development of capabilities for propagation of errors in composition as a function of depletion, development of automated temperature interpolation capability, and representation of the neutronic effects of thermal, hydraulic, and structural variations.

#### Development and Application of Evaluation Methodologies

- Develop an economic model for evaluation of actinide management services that can be provided by Generation IV systems operated with either an open or closed fuel cycle. These services can range from consumption of existing stocks of actinides to creation of excess fissile materials to fuel expansion of nuclear generation capacity.

- Contribute to further development and application of economic models under development by the GIF Economic Modeling Working Group (EMWG). Of particular interest are contributions to modeling the economics of non-electricity energy products (e.g., hydrogen generation) and optimizing the increment of plant generation-capacity addition.
- Develop risk-based and technology-independent safety criteria that may be used as a basis for regulatory review and approval of Generation IV systems.
- Develop comprehensive criteria for evaluating sustainability of nuclear energy systems in comparison to alternative energy supply options. Account for economic, environmental, technical, and societal dimensions of sustainability.
- Contribute to further development and application of the GIF proliferation resistant and physical protection (PR&PP) methodology. Contributions may include systematic selection and importance weighting of proliferation and security threats; further detailing of scenarios, pathways, and impediments for selected Gen IV systems and postulated threats; development of quantitative approaches for evaluating the PR&PP measures defined by the GIF expert group; development of additional or alternative PR&PP measures; and development of approaches for aggregating the measures into an overall indicator of proliferation resistance or physical protection.

## **2.6 Crosscutting Materials Development for Advanced Reactors**

The listing of some R&D needs below is organized according to programmatic activity categories.

### **Crosscutting Materials for Radiation Service**

- Perform design of facilities for both low-flux and high-flux, high-temperature irradiations.
- Initiate low-dose scoping irradiations of commercial, near-commercial, and advanced materials and their PIE to complete selection of primary reactor pressure vessel (RPV) candidate materials based on screening irradiation experiments.

### **Crosscutting Materials for High-Temperature Service**

- Complete the establishment of an initial database for candidate materials for high-temperature and radiation service for all Gen IV reactor systems.
- Identify deficiencies in high-temperature materials needed for codification.
- Perform scoping studies of mechanical properties for high-temperature materials.
- Perform joining and combined-effects high-temperature screening studies on commercial and near-commercial alloys and advanced high-temperature materials.

### **Crosscutting Task on Modeling and Microstructural Analysis**

- Prepare an integrated report prioritizing microstructural modeling needs for Generation IV reactors and identify needed special-purpose experiments.

- Evaluate models for the nucleation phase of the significant extended defects produced under irradiation.
- Evaluate overall microstructural evolution under low- and high-temperature irradiation, including results from preliminary modeling studies and microstructural characterization.
- Initiate microstructural model development in critical areas.

#### Crosscutting Task on High Temperature Design Methodology

- Develop interior constitutive equations for modified 9Cr-1Mo steel (Grade 92) and Alloy 617

#### NGNP-Specific Materials Research

- Complete scoping irradiations of NGNP structural alloys for RPV and internals applications.
- Perform a time-independent mechanical properties evaluation of commercial and near-commercial alloys for NGNP service
- Complete an initial assessment and provide materials use guidelines for carbon-carbon (C-C) composites, insulator, metallic reactor internals, bolting, and heat exchanger materials in the NGNP gaseous environment.
- Transition constitutive equation development to candidate NGNP pressure boundary materials and NGNP very-high-temperature component materials.
- Develop initial simplified high-temperature design rules for use in the preliminary design of NGNP components.
- Perform uniaxial and biaxial creep-fatigue tests and the development of a creep-fatigue damage model for modified 9Cr-1Mo steel (Grade 92) and Alloy 617.
- Perform structural tests of Alloy 617 models at very high temperatures.
- Use interior constitutive equations to develop isochronous stress-strain curves and other predicted behavioral representations for modified 9Cr-1Mo steel (Grade 92) and Alloy 617.
- Propose creep-fatigue criteria for modified 9Cr-1Mo steel (Grade 92) and Alloy 617.
- Complete Alloy 617 confirmatory structural tests, and initiate testing of models for other key NGNP structural materials.
- Complete preliminary characterization of baseline physical and mechanical properties of NGNP candidate graphites.
- Complete graphite physical and mechanical properties evaluations for NGNP.

- Complete preliminary graphite oxidation effects studies of NGNP graphites.
- Complete preliminary irradiation effects studies of NGNP graphites.
- Complete design and construction of NGNP graphite irradiation creep capsules.
- Complete ASTM standard materials specification development in support of NGNP graphite.
- Complete evaluation of as-received properties of candidate C-C composites for control rods, bolting, and insulation materials for NGNP.
- Initiate design and construction of NGNP materials compatibility test facilities and establish required test matrices.
- Initiate emissivity testing for NGNP RPV.
- Initiate mechanical testing of pressure boundary and insulation materials in the NGNP gaseous environment.

#### GFR-Specific Materials Research

- Initiate materials compatibility studies of ODS ferritic-martensitic steels, Nb- and Mo-base alloys, and ceramics including Nb- and Mo-base cermets with impure helium for GFR.
- Initiate materials compatibility studies with super-critical CO<sub>2</sub> in the temperature range of 400 to 650°C for GFR.
- Initiate irradiations of candidate GFR internals structural materials in a fast-spectrum environment.

#### SCWR-Specific Materials Research

- Evaluate capabilities of suppliers for thick-section RPV for SCWR and demonstrate fabrication capabilities.
- Perform initial unirradiated mechanical properties testing of candidate materials for SCWR.
- Begin scoping irradiation experiments for reactor internals candidate materials for SCWR.
- Complete compilation of available information on solubility of SCWR power conversion systems candidate materials in supercritical steam.
- Perform initial corrosion and SCC screening tests in supercritical water for SCWR.

- Initiate corrosion fatigue testing for SCWR pump and power conversion systems materials in supercritical water.
- Initiate compilation of available information and perform additional measurements required on solubility of SCWR candidate materials in supercritical steam.
- Initiate evaluation of factors affecting condensation and stability of corrosive species in SCWR power conversion systems.

#### LFR-Specific Materials Research

- Perform scoping studies of preliminary LFR candidate materials for corrosion resistance.
- Initiate scoping studies of surface treatments for controlling corrosion in LFR environments.
- Initiate an assessment of creep and aging mechanisms in LFR materials.
- Initiate an assessment of surface protection mechanisms in LFR materials.
- Complete a preliminary selection of primary candidate materials for LFR system.
- Initiate an assessment of mechanical and corrosion properties of primary candidate LFR materials in as-received condition.
- Initiate an aging and irradiation assessment of primary candidate LFR materials.

### **2.7 Energy Conversion**

The listing of some R&D needs below is organized according to programmatic activity categories.

#### Supercritical CO<sub>2</sub> Power Conversion Cycles

- The compression stage of a supercritical CO<sub>2</sub> cycle involves operation near the critical point of CO<sub>2</sub>. Examine analytical tools for S- CO<sub>2</sub> power conversion cycles and develop improved models for near critical point operation, including working fluid properties, thermodynamic analysis and turbomachinery design.
- Develop a simulation model to address S-CO<sub>2</sub> dynamic response to startup and off normal operation. Investigate inventory or other control mechanisms for system operation. Develop innovative load-following approaches as an alternative to inventory control.
- Identify requirements for a small scale experiment to demonstrate the key technology and operational features of the supercritical CO<sub>2</sub> cycle. Perform analysis to define experiment scale and verify performance.
- Evaluate the use of radial turbomachinery, especially compressors, in place of axial compressors for the S- CO<sub>2</sub> cycle.

- Develop and test shaft seal and bearing designs for use in S-CO<sub>2</sub> bearing tribology tests.
- Evaluate the S-CO<sub>2</sub> cycle as a bottoming cycle on the VHTR thermochemical H<sub>2</sub> unit; evaluate a bottoming cycle for S-CO<sub>2</sub> cycles; devise a practical CO<sub>2</sub> condensing cycle version.
- Evaluate costs and benefits of using inverters to allow non-synchronous shaft rotational speeds for S-CO<sub>2</sub> turbines.
- Perform steady state and transient pressure/ thermal/ combined stress analyses of turbines, compressors and other key components for supercritical CO<sub>2</sub> conceptual designs.
- Evaluate 2 and 3 shaft turbomachinery layouts to compare to single and multiple shaft configurations.

#### High Temperature Brayton Cycle Studies.

- Develop innovative heat exchanger designs for interstage heating and cooling for high temperature inert gas Brayton cycles that minimize temperature and pressure drops for both liquid-gas and gas to gas heat exchangers.
- Develop algorithms for optimization of Brayton cycle configurations, efficiency and cost to allow comparison of advanced cycle configurations.
- Investigate hybrid (hydrogen and electrical) plant configurations to evaluate economic and operational issues with plants that could produce hydrogen or electricity based on market demands. Compare economic implications of hybrid and dedicated plant configurations.
- Perform analyses to evaluate experimental requirements for a viable small scale high temperature He Brayton cycle test to demonstrate efficiency improvements for interstage heated, cooled or other cycle configurations. Develop a preliminary design for major components.
- Investigate single vs. multiple shaft configurations and non-synchronous shaft rotational speeds using invertors and evaluate economic and operational implications.
- Perform analyses to compare direct vs. indirect cycle approaches for high temperature reactors. Identify engineering approaches to minimize or mitigate efficiency, cost implications for indirect cycles, or mitigate operational and maintenance impacts of direct cycles.

### **3. Nuclear Hydrogen Initiative**

#### **3.1 Thermochemical Cycles**

The listing of some R&D needs below is organized according to programmatic activity categories.

### Flowsheet Methodology

- Evaluate and compare flowsheet analysis approaches for thermochemical cycles and develop a consistent analysis approach for comparison of processes with uncertainties in thermodynamic data and process definition.
- Assess thermodynamic and physical property data base assumptions used in current modeling programs and identify gaps and R&D needs.
- Assess sensitivities to data uncertainties and develop an approach for estimating potential impacts.

### Thermochemical Cycle Analysis

- Identify alternative thermochemical cycles (not current baseline) for nuclear hydrogen production that have potential for higher efficiency, lower temperature operation or are less complex, but are not presently characterized to determine viability.
- Perform flowsheet analyses to characterize process(es), in order to allow assessment of performance potential and preliminary comparison with baseline cycles.
- Identify basic thermodynamic data or laboratory experiments for alternative cycles that are needed to improve assessments.

### Sulfur-Iodine Cycle

- Investigate alternative approaches for the concentration and decomposition of sulfuric acid that utilize heat more efficiently, using flowsheet models.
- Investigate alternative approaches for the distillation of HI from iodine and water solution, such as extractive distillation using  $\text{H}_3\text{PO}_4$  or electrodialysis for concentration, that reduce the amount of water recycle or increase the yield from HI decomposition and increase efficiency.
- Develop innovative heat exchanger approaches for the high temperature sulfuric acid sections that minimize materials corrosion impact on heat exchanger viability by using sacrificial materials, direct contact heat exchange or other engineering approaches to reducing overall materials requirements.
- Investigate control issues for closed cycle thermochemical systems and develop preliminary models to examine startup, off normal, and shutdown issues for complex thermochemical plants. Develop preliminary control algorithms for closed loop operation of thermochemical cycles.

### Membranes for Sulfur Cycles

- Perform an assessment of membrane technologies potentially applicable to key separation or concentration stages of sulfur cycles that could improve efficiency or reduce complexity. Identify membrane options and potential performance or cost benefits.



- Perform a preliminary assessment of promising alternative cycles, such as those listed in the NHI R&D Plan, to identify areas where improvements in key separations could provide improved performance or reduce cycle complexity.

#### Hybrid Sulfur

- Investigate electrolytic cell design and performance for the electrolysis of SO<sub>2</sub> and water. Identify design, operational conditions, or materials that reduce electrical losses. Also identify modular designs for maximizing economy of scale.
- Investigate scaling approaches for large hybrid hydrogen plants, including the implications of operational strategies for co-generation of hydrogen with lower cost off peak electricity to reduce overall production costs.
- Investigate improved or alternative materials for anodes, cathodes, and membranes materials for H<sub>2</sub>SO<sub>3</sub> electrolysis.
- Develop conceptual designs and economic optimization algorithms for hybrid sulfur plants to be used as the basis for cost assessments.

#### Heat Exchanger Design and Development for Sulfur Cycles

- Develop innovative heat exchanger designs for high temperature heat transfer to corrosive liquids or gases, and perform engineering analysis to assess design requirements and performance for this application.
- Perform thermal, structural and flow analysis for advanced materials heat exchanger concepts, such as SiC and graphite based units, to define high temperature strength and compatibility issues for ceramic and composite based approaches.

#### Materials Requirements and Testing for Sulfur Cycles

- Investigate high temperature materials for use in corrosive environments, including superalloys, refractory metals, high silicon steels, ceramics and graphite based materials. Define performance potential for sulfur cycles and identify physical property and compatibility testing requirements.
- Develop materials testing approaches to extract maximum long term corrosion behavior from limited data.
- Investigate advanced coatings for high temperature corrosion resistance. Identify promising coating options and evaluate the potential for sulfur cycle heat exchangers.

#### Calcium Bromide Cycles

- Investigate alternative electrolytic systems (with Br<sup>-</sup> as the charge carrier) for the decomposition of HBr for hydrogen generation in the Ca-Br cycle and develop a conceptual design to support cost and performance projections.
- Investigate systems for the separation of HBr from H<sub>2</sub>O and H<sub>2</sub>.
- Investigate the formation of unsupported CaBr<sub>2</sub> from CaO with Br<sub>2</sub>.
- Identify innovative approaches to improve the cyclic performance and stability of CaO-CaBr<sub>2</sub> solid-gas reaction beds. Define lab scale test requirements to demonstrate bed stability for cyclic operation.
- Determine the recovery of O<sub>2</sub> with trace levels of Br<sub>2</sub> and evaluate the impacts of Br<sub>2</sub> release to environment if O<sub>2</sub> is used for publicly owned treatment systems for water.

### **3.2 High Temperature Electrolysis**

The listing of some R&D needs below is organized according to programmatic activity categories.

#### **Commercial System Definition**

- Define major components of electrolytic systems, starting with the bench-scale and then progressing to lab-scale, pilot-scale, engineering-scale and finally to the demonstration level.

#### **Flowsheet Analysis**

- Perform a flowsheet analysis for the pilot-scale (50 kW) and engineering-scale (500 kW) experiments. These flowsheet analyses will be instrumental in determining the gas consumption and flow rates, the recycling of heat and materials, the utilities required, the operating conditions, and even determining the location of the pilot-scale experiment.

#### **Engineering Analysis**

- Determine the design requirements and feasible stack cell dimensions for each scale (pilot-scale, engineering-scale, and demonstration-scale). For instance, high pressure operation, optimization of heat recovery, long-term material compatibility with hydrogen, and product purification may only be important at larger scales. Feed stream pre-heating and stack heating are also scale-dependent. Include in this task infrastructure requirements, footprints, sizing of components, heat rejection and recovery needs, instrumentation, data acquisition and process control requirements, materials of construction, design optimization, preliminary drawings, and permitting requirements (ES&H).

#### **HTE Experimental System**

##### **Conceptual Design**

- Define lab-scale testing objectives, develop Process & Instrumentation Diagrams (P&ID), instrumentation requirements, flow configuration, materials of construction, operating conditions, flow rates, and insulation requirements.

### Final Design

- Collaborate in materials and instrumentation procurement, fabricate specialized hardware, assemble the experimental setup, develop the required data acquisition system, and begin preliminary testing. Stacks will be provided under subcontract with Ceramtec.

### Cell/stack Operation

- Conduct stack testing, with parameters to include feed gas flow rates and composition, current density, operating temperature, and stack materials of construction (2 or 3 stacks to be tested).

## **3.3 Reactor-Hydrogen Production Process Interface**

The listing of some R&D needs below is organized according to programmatic activity categories.

### Nuclear Hydrogen System Design Studies

System design studies for the system interface and balance-of-plant areas address plant configuration options for both thermochemical and high-temperature electrolysis systems, safety and isolation issues for the coupled plants, and assessment of applicable codes and standards. Since these studies define fundamental options for the nuclear hydrogen plant configuration and nuclear interface, they must be addressed early in the FY 2005 to 2007 time frame.

- Perform hydrogen plant configuration studies to define configuration options and the operational conditions and requirements for the hydrogen plant subsystems. The isolation approach for nuclear and hydrogen production systems, both thermochemical and electrolytic processes, has performance and economic implications that need to be addressed at the earliest possible stage. These studies define options and tradeoffs for the optimum coupling of the nuclear and chemical systems.
- Perform system interaction studies to define safety and isolation issues arising from system level considerations and from functional and physical coupling of the nuclear and hydrogen plants. Nuclear hydrogen production systems will require a new or modified framework for regulation. Identification of information on combined plant operational requirements that could impact system design and preliminary definition of accident categories may be important in process evaluation. The tasks that should be addressed include assessment of regulatory requirements, definition of separation and isolation criteria, and preliminary plant safety studies.
- Compile the applicable codes, standards, and guidelines for the nuclear plant and the hydrogen production processes of interest, and identify any issues. Numerous codes, standards, and guidelines are applicable to H<sub>2</sub> and O<sub>2</sub>, but no definitive compilation has been identified.

- Define the design and performance requirements determined by hydrogen production process characteristics and high-temperature reactor capabilities to establish conditions for balance-of-plant systems.

### Heat Exchanger Design Studies

High-temperature heat exchangers that transfer thermal energy to chemical processes or steam at elevated temperature are critical components. Operational conditions for the interface heat exchangers are challenging. The heat exchanger for the Sulfur-Iodine and Hybrid Sulfur processes require decomposition of sulfuric acid at more than 850°C and up to several megaPascals (MPa). Heat exchangers for the high-temperature electrolysis process will actually be steam generators producing steam at up to 950°C and up to 5 MPa.

- Perform thermal analyses between intermediate loop and process conditions to define operational requirements for heat exchangers for the range of candidate cycles to support heat exchanger design studies.
- Perform heat exchanger design studies to explore innovative heat exchanger design approaches that could potentially mitigate temperature or lifetime requirements. A range of heat exchanger design approaches can be considered (tube/shell, printed circuit) that involve differing materials and fabrication issues. Heat exchanger viability is an essential consideration in the selection of a pilot plant hydrogen process.
- Perform high-temperature materials test programs to demonstrate performance and lifetime under prototypic conditions. Based on the operating conditions and requirements for process-specific heat exchangers, this task will identify and initiate materials testing programs for the candidate cycles. This activity also addresses fabrication issues for heat exchanger designs and will require industrial participation in their design and fabrication. Scaled demonstration testing is required for selected heat exchanger systems.

### Intermediate Heat Transfer Loop

Intermediate loop studies will define the interface with the reactor heat source, including operational conditions, materials, and controls. The selection of the heat transfer medium and transfer line configuration and materials are key technologies that impact both reactor and process design choices.

- Perform an analysis to determine the optimal medium/fluid for the intermediate heat transfer loop. This selection impacts plant configuration, separation distance decisions, heat exchanger design, and materials selection. The medium must be compatible with temperatures up to 1000°C, pressures of several MPa, and reasonable pumping/circulating requirements, as well as chemical compatibility with heat transfer loop materials. Helium, molten salts, and liquid metal have been identified as potential candidates for the heat transfer medium.
- Perform thermal analysis and materials development studies for the intermediate heat transfer loop transfer lines. Materials development will be required for piping and seals, circulator (pumps or blowers), valves, and structural materials (900 to 1000°C range). The technology gaps for the use of helium involve equipment sizes and blower operating

costs. Materials for molten salt structural materials, pumps, and valves have a technology gap between previously demonstrated use at approximately 700°C and the required range of 900 to 1000°C. The technology gaps in the use of liquid metals, which include pumping, high-temperature valve development and material compatibility issues, lie between 450°C and the required range of 900 to 1000°C.